

Supporting Information

Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite

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Table S1. Average Fe^{2+} -O bond length ($R_{\text{Fe}^{2+}\text{-O}}$) and Si-O bond length ($R_{\text{Si}\text{-O}}$) derived from the static calculations on Si@EP Fe_2O_3 , with respect to $R_{\text{Fe}^{2+}\text{-O}}$ of 2.11 Å in e@EP Fe_2O_3 . Units are Å.

	Fe1	Fe2	Fe3	Fe4	Fe5	Fe6	Fe7	Fe8
$R_{\text{Fe}^{2+}\text{-O}}$	2.135	2.123	2.135	2.135	2.128	2.128	2.127	2.131
$R_{\text{Si}\text{-O}}$	1.849	1.855	1.849	1.849	1.851	1.851	1.851	1.847

Table S2. Three neighboring Fe²⁺-Fe distances (R_1 , R_2 , and R_3 , units are Å) extracted from the AIMD trajectory at 300 K for e@EP Fe₂O₃, averaged over each stage defined in Figure 2, compared to the static values (in bold) at 0 K.

Stage	R_1	R_2	R_3	Stage	R_1	R_2	R_3	Stage	R_1	R_2	R_3
Fe1	Fe6	Fe8	Fe5		Fe6	Fe7	Fe8	Fe6	Fe2	Fe1	Fe3
	2.91	2.97	2.99		2.91	2.97	2.99		2.91	2.97	2.99
Fe1-I	Fe5	Fe6	Fe8		Fe5	Fe8	Fe7		Fe2	Fe1	Fe3
	2.96	2.96	2.97		2.91	2.97	2.99		2.96	2.96	2.96
Fe1-II	Fe6	Fe8	Fe5		Fe5	Fe8	Fe7		Fe1	Fe3	Fe2
	2.96	2.96	2.96		2.96	2.96	2.96		2.95	2.96	2.96
Fe1-III	Fe6	Fe8	Fe5		Fe2	Fe4	Fe1		Fe4	Fe2	Fe3
	2.96	2.96	2.96		2.91	2.97	2.99		2.91	2.97	2.99
Fe2	Fe7	Fe6	Fe5		Fe4	Fe1	Fe2		Fe4	Fe2	Fe3
	2.91	2.97	2.99		2.95	2.96	2.96		2.96	2.96	2.96
Fe2-I	Fe6	Fe5	Fe7		Fe1	Fe2	Fe4		Fe1	Fe4	Fe3
	2.96	2.97	2.97		2.95	2.96	2.96		2.91	2.97	2.99
Fe2-II	Fe7	Fe6	Fe5		Fe4	Fe2	Fe1		Fe1	Fe4	Fe3
	2.96	2.96	2.96		2.75	2.92	3.02		2.96	2.96	2.96

^① an exception occurs in Fe5-III where the collected data are too few due to a very short duration of the EP stays in this stage.

Table S3. Three neighboring Fe²⁺-Fe distances (R_1 , R_2 , and R_3 , units are Å) extracted from the AIMD trajectory at 300 K for Si@EP Fe₂O₃, time-averaged over each stage defined in Figure 3, and compared to the static values (in bold) at 0 K.

Stage	R_1	R_2	R_3	Stage	R_1	R_2	R_3	Stage	R_1	R_2	R_3
Fe8	Fe4	Fe3	Fe1		Fe4	Fe3	Fe2		Fe8	Fe7	Fe6
	2.89	2.95	2.98		2.90	2.97	3.01		2.90	2.97	3.01
Fe8-I	Fe1	Fe3	Fe4		Fe4	Fe3	Fe2		Fe8	Fe7	Fe6
	2.94	2.95	2.95	Fe7-I	2.92	2.96	3.02		2.93	2.95	2.95
Fe8-II	Fe4	Fe3	Fe1		Fe4	Fe3	Fe2		Fe8	Fe5	Fe7
	2.94	2.95	2.95	Fe7-II	2.91	2.96	3.02		2.91	2.95	2.98
Fe8-III	Fe4	Fe3	Fe1		Fe4	Fe3	Fe2		Fe8	Fe5	Fe7
	2.95	2.95	2.95	Fe7-III	2.92	2.96	3.02		2.95	2.95	2.96
Fe8-IV	Fe4	Fe3	Fe1		Fe4	Fe3	Fe2		Fe7	Fe5	Fe8
	2.94	2.95	2.95	Fe7-IV	2.91	2.96	3.01		2.94	2.95	2.97
Fe5	Fe1	Fe4	Fe2		Fe8	Fe6	Fe5		Fe7	Fe5	Fe8
	2.90	2.97	3.01		2.91	2.95	2.98		2.92	2.95	2.96
Fe5-I	Fe1	Fe4	Fe2		Fe6	Fe8	Fe5		Fe7	Fe5	Fe8
	2.93	2.96	3.01	Fe1-I	2.93	2.95	2.95		2.92	2.95	2.98
Fe6	Fe3	Fe1	Fe2		Fe8	Fe7	Fe6		Fe8	Fe5	Fe7
	2.90	2.97	3.01		2.91	2.95	2.98		2.94	2.94	2.96
Fe6-I	Fe3	Fe1	Fe2		Fe6	Fe7	Fe8		Fe7	Fe6	Fe5
	2.92	2.97	3.01	Fe3-I	2.93	2.93	2.95		2.96	3.01	3.02
Fe6-II	Fe3	Fe1	Fe2		Fe6	Fe7	Fe8				
	2.92	2.96	3.01	Fe3-II	2.93	2.95	2.97				

Table S4. Fe²⁺-O bond lengths ($\langle R_{\text{Fe}2+\text{-O}} \rangle$) time-averaged over the stages of Fe²⁺, and Fe³⁺-O bond lengths ($\langle R_{\text{Fe}3+\text{-O}} \rangle$) time-averaged over the stages of Fe³⁺, derived from the AIMD simulations on e@EP and Si@EP Fe₂O₃, respectively, with the standard deviation in parentheses reflecting the magnitude of thermal fluctuations. Definition of the stages is shown in Figures 2 and 3, and units are Å.

	Fe1	Fe2	Fe3	Fe4	Fe5	Fe6	Fe7	Fe8
e@EP Fe ₂ O ₃								
$R_{\text{Fe}2+\text{-O}}$	2.118 (0.022)	2.118 (0.023)	-	2.118 (0.023)	2.118 (0.023)	2.118 (0.023)	2.119 (0.023)	2.118 (0.021)
$R_{\text{Fe}3+\text{-O}}$	2.047 (0.019)							
Si@EP Fe ₂ O ₃								
$R_{\text{Fe}2+\text{-O}}$	2.128 (0.029)	-	2.130 (0.025)	2.129 (0.027)	2.132 (0.024)	2.130 (0.022)	2.131 (0.023)	2.135 (0.023)
$R_{\text{Fe}3+\text{-O}}$	2.059 (0.028)	2.053 (0.020)	2.060 (0.028)	2.060 (0.028)	2.059 (0.020)	2.059 (0.019)	2.060 (0.019)	2.058 (0.019)

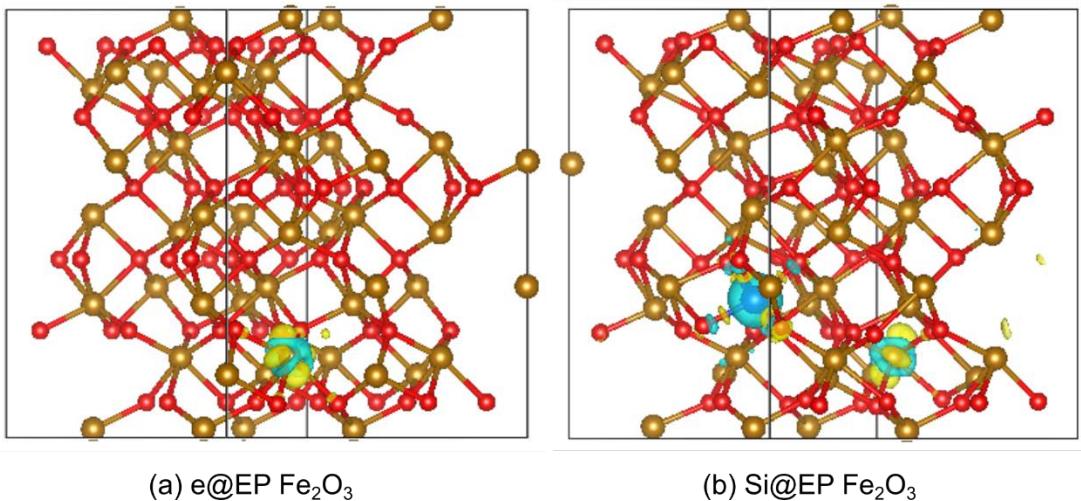


Figure S1. Difference charge density for the two EPs of Fe_2O_3 before and after an excess electron injection or a foreign Si atom doping, demonstrating that the EPs are generated in Fe_2O_3 . Accumulation and depletion of electron charge are shown in yellow and cyan, respectively, with the iso-value of $0.01 \text{ e}/\text{bohr}^3$. Charge depletion around the Si dopant in (b) arises from the different valence electrons for Si compared to Fe, namely, $\text{Si } 3s^23p^2$ and $\text{Fe } 3d^64s^2$.

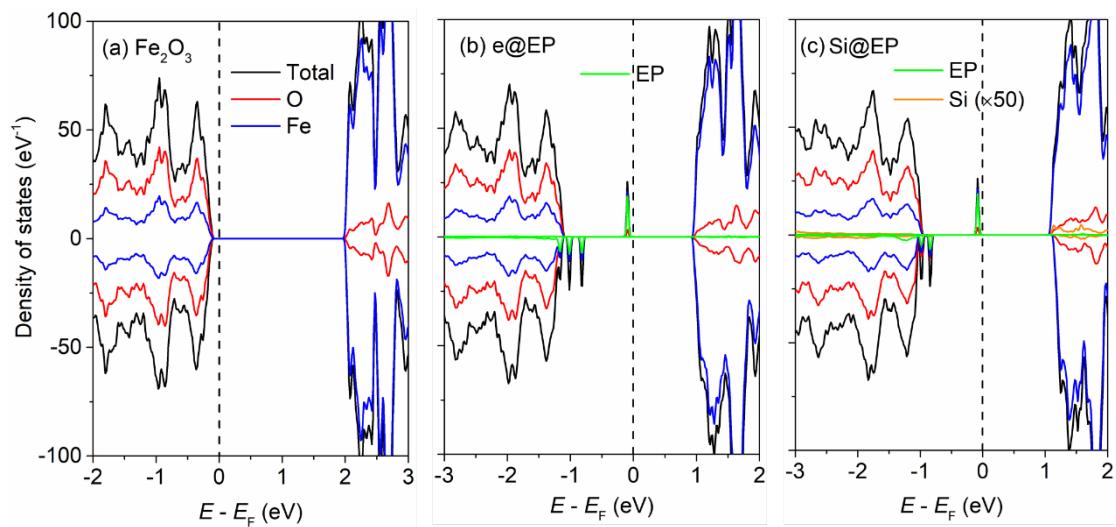


Figure S2. Density of states for (a) pure Fe_2O_3 , (b) $e@\text{EP}$, and (c) $\text{Si}@\text{EP}$ Fe_2O_3 . Formation of EPs in Fe_2O_3 gives rise to highly localized electronic states in the band gap.

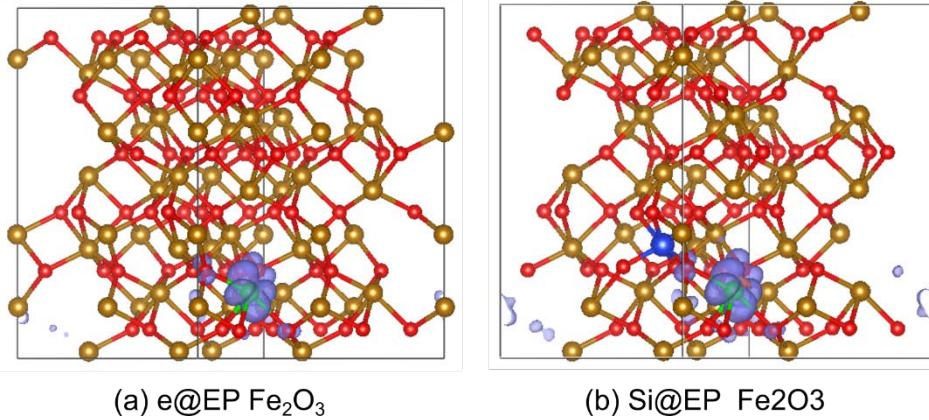


Figure S3. Charge density of the EP state in (a) e@EP and (b) Si@EP Fe_2O_3 , depicted in dark blue with the iso-value of 0.002 e/ bohr^3 .

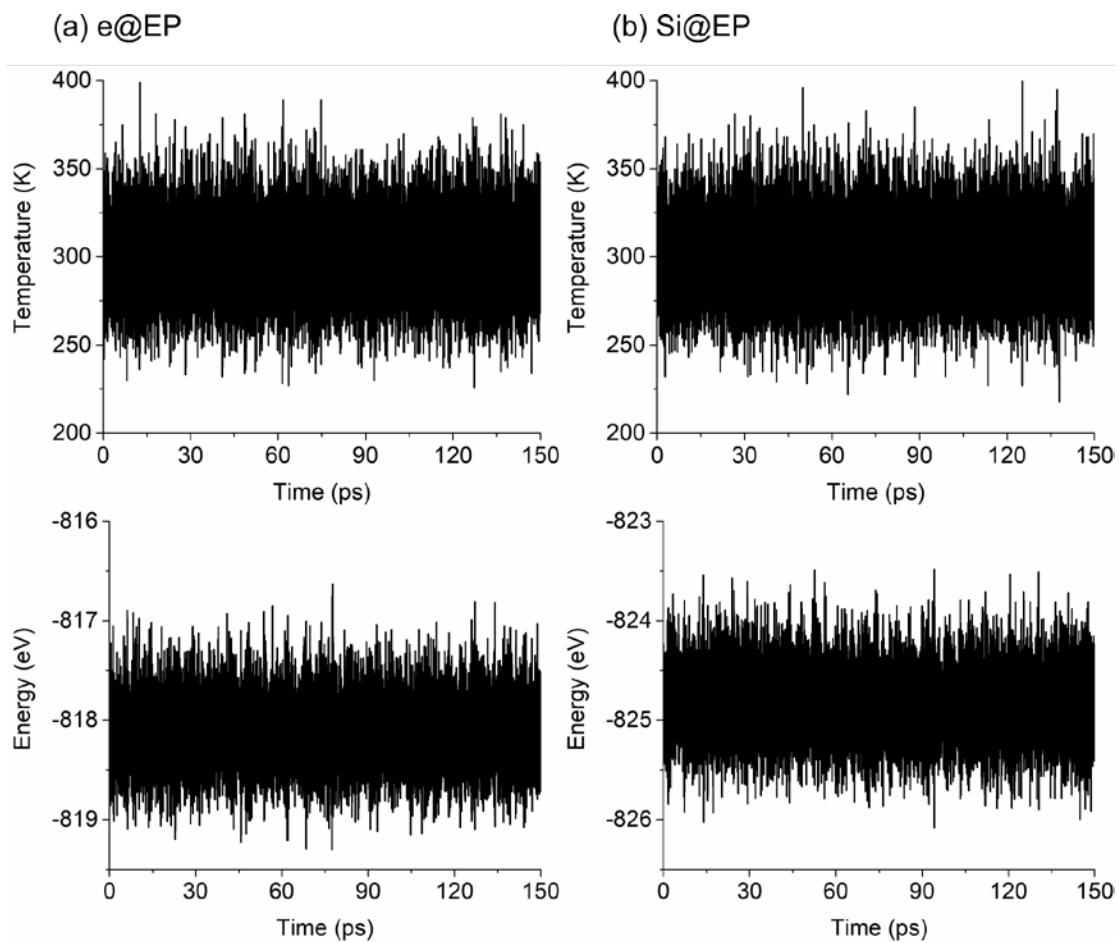


Figure S4. Temperature (upper panels) and energy (lower panels) as functions of time extracted from the AIMD trajectories for (a) e@EP and (b) Si@EP Fe_2O_3 . Note that the average energy of Si@EP Fe_2O_3 is lower by ~43 meV after 55 ps.

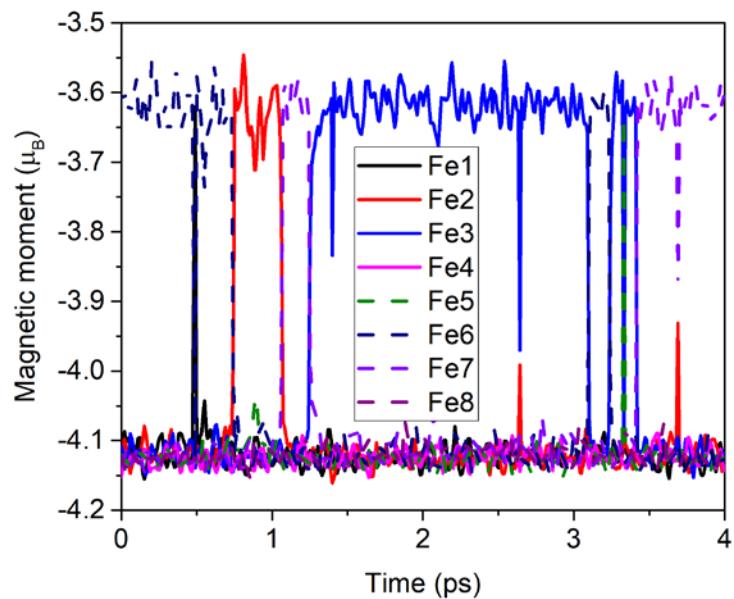


Figure S5. Local magnetic moments on the eight Fe ions of the Fe bilayer in the basal plane for e@EP Fe_2O_3 at 600 K as functions of the simulation time. The EP hops 9 times during the simulation time of 4 ps, significantly faster than the EP at 300 K.

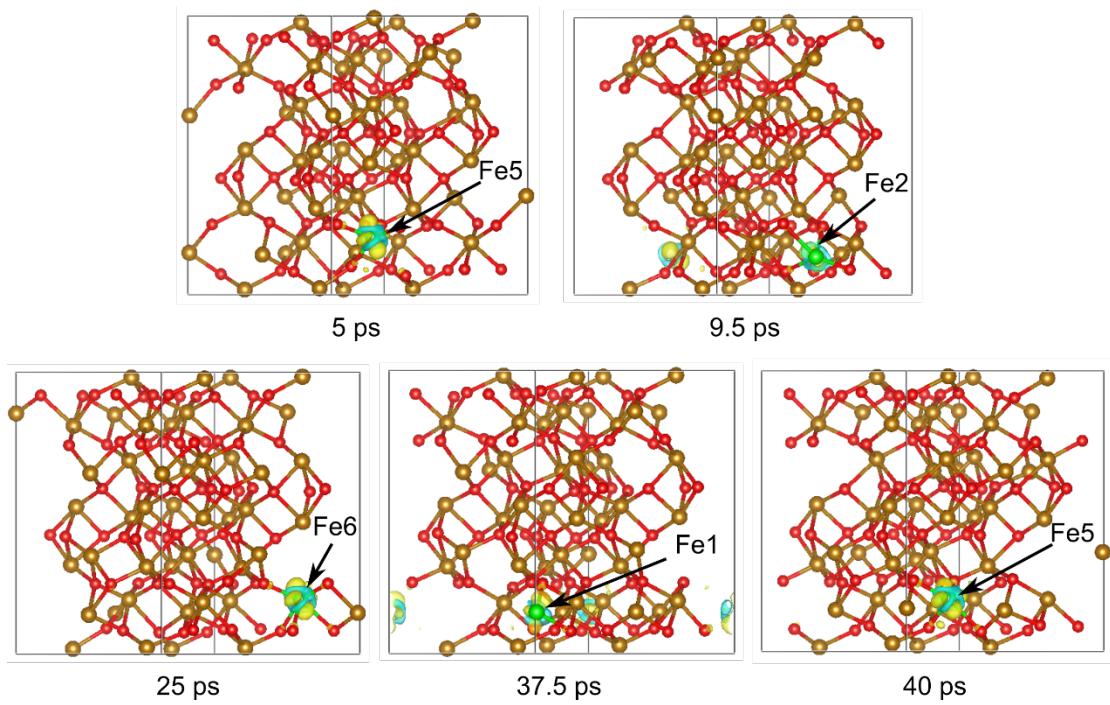


Figure S6. Difference charge density for snapshots chosen from the first 40 ps of the 150 ps trajectory for e@EP Fe₂O₃ at 300 K, depicted with the iso-value of 0.01 e/ bohr³.

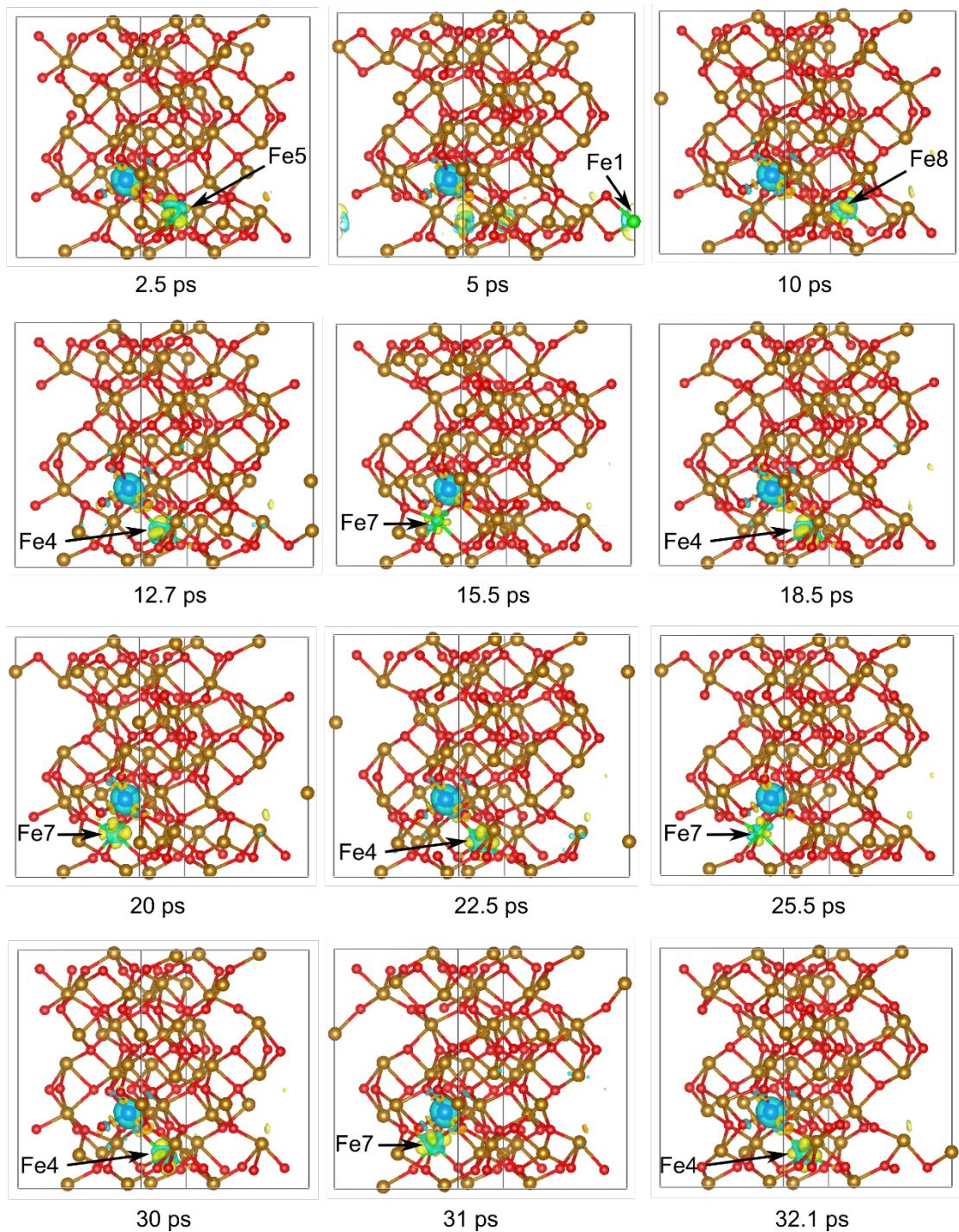


Figure S7. Difference charge density for snapshots chosen from the first 35 ps of the 150 ps trajectory for Si@EP Fe₂O₃ at 300 K, depicted with the iso-value of 0.01 e/bohr³.

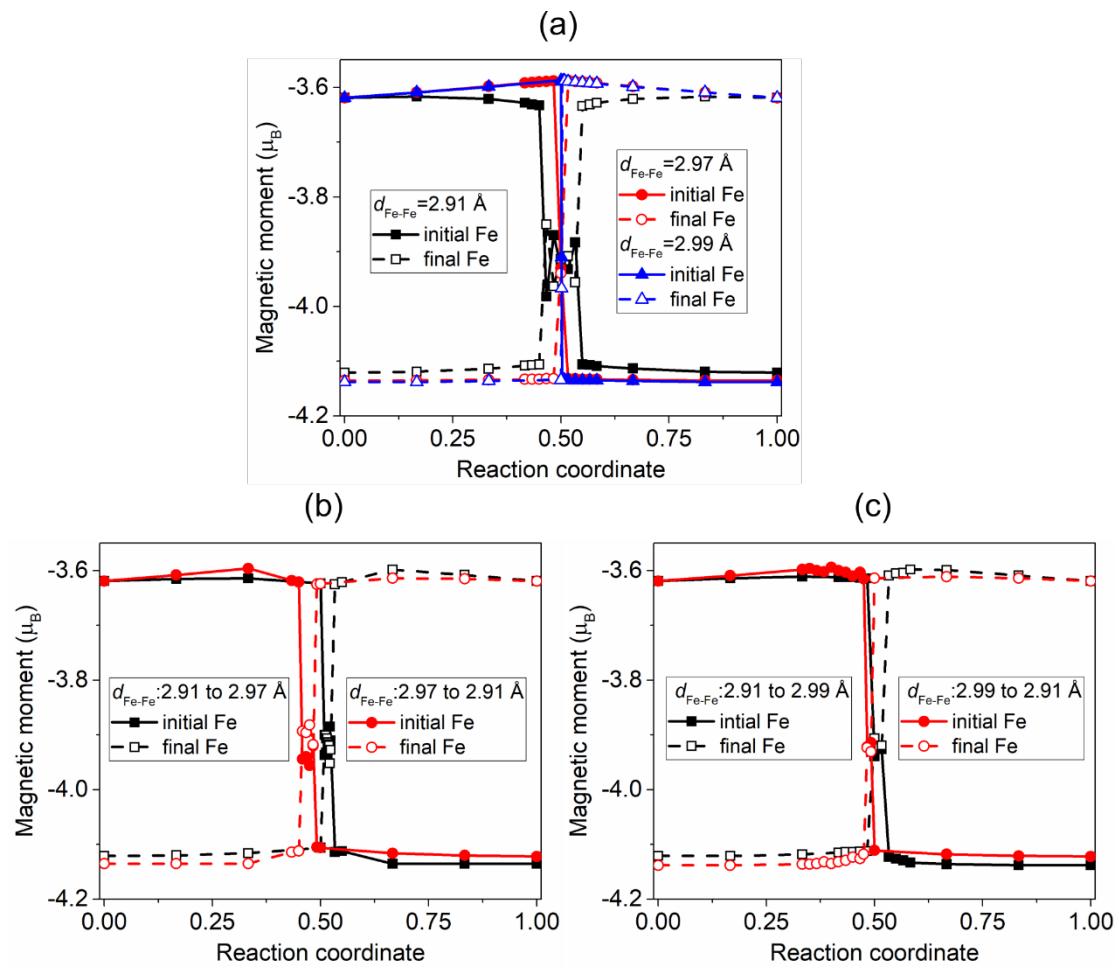


Figure S8. Local magnetic moment on the two Fe ions which are involved in the EP hopping along the reaction path in e@EP Fe_2O_3 between (a) equivalent and (b, c) inequivalent initial and final coordinates. The reaction path is defined by Equation (3).

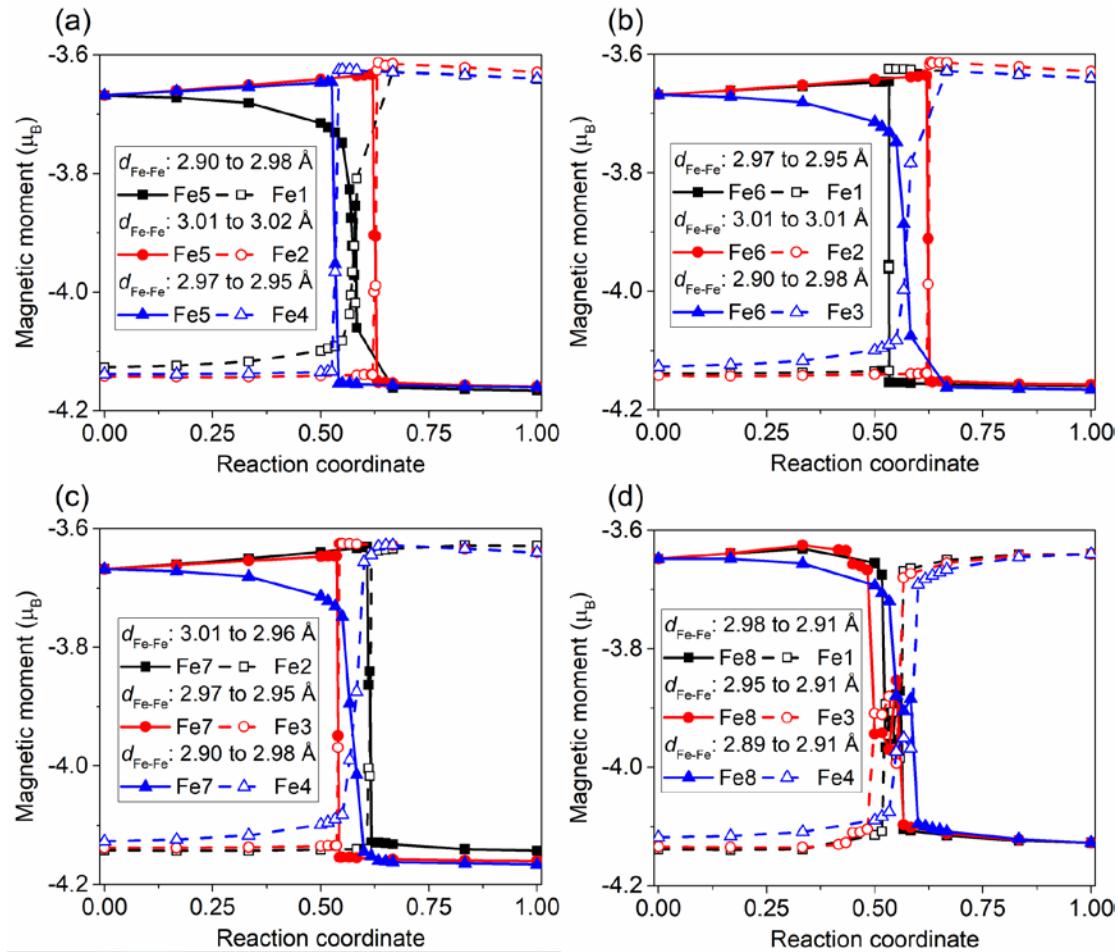


Figure S9. Local magnetic moments on the two Fe ions in Si@EP Fe₂O₃ which are involved in the EP transfer along the reaction path defined by Equation (3), with the initial coordinate on (a) Fe5, (b) Fe6, (c) Fe7 and (d) Fe8, and the final coordinate on their three nearest Fe neighbors.

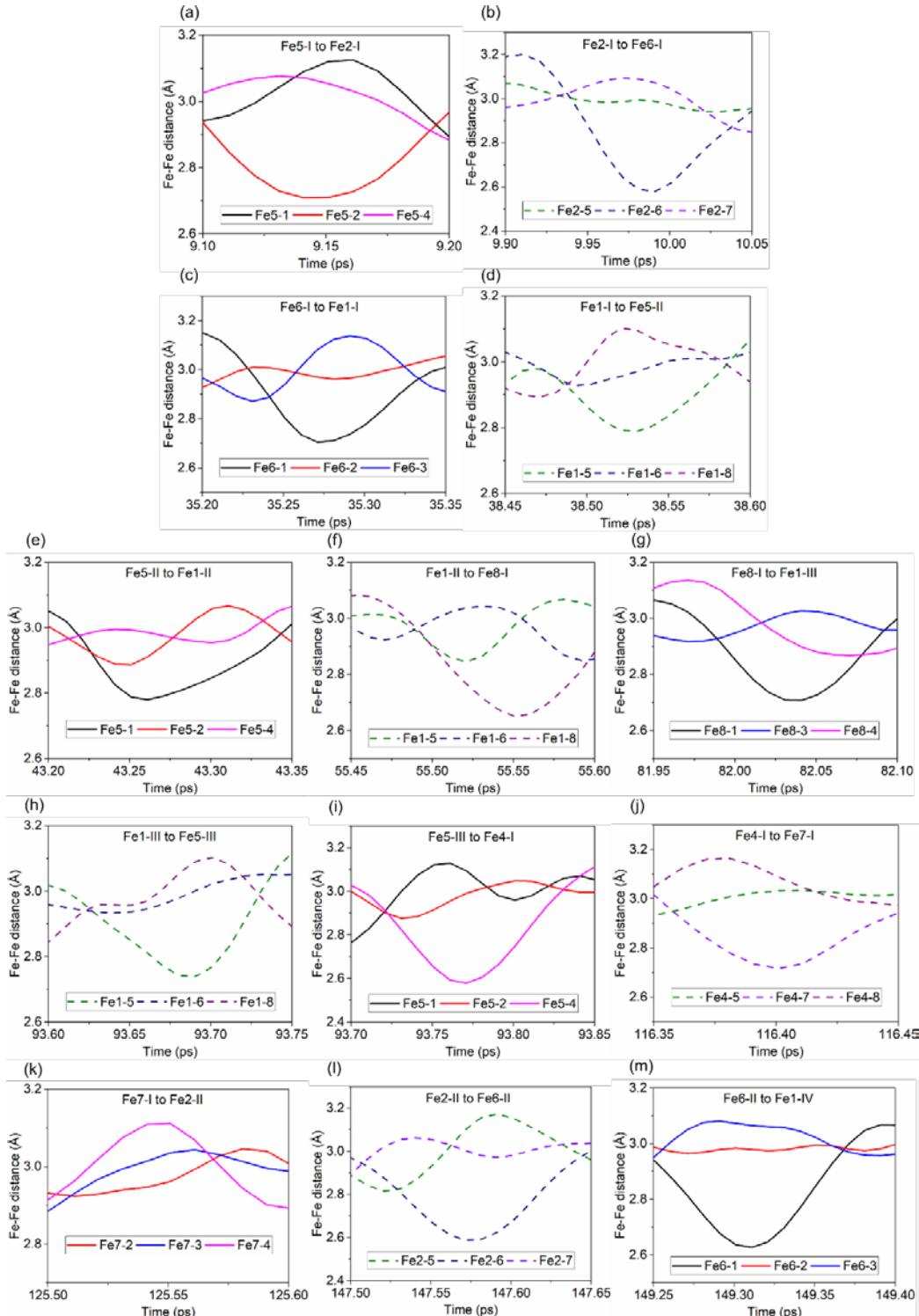


Figure S10. Three nearest Fe-Fe distances in the temporal windows of 0.1-0.15 ps for each EP hopping in e@EP Fe₂O₃, extracted from the AIMD trajectory of 150 ps: **(a)** Fe5-I to Fe2-I, **(b)** Fe2-I to Fe6-I, **(c)** Fe6-I to Fe1-I, **(d)** Fe1-I to Fe5-II, **(e)** Fe5-II to Fe1-II, **(f)** Fe1-II to Fe8-I, **(g)** Fe8-I to Fe1-III, **(h)** Fe1-III to Fe5-III, **(i)** Fe5-III to Fe4-I, **(j)** Fe4-I to Fe7-I, **(k)** Fe7-I to Fe2-II, **(l)** Fe2-II to Fe6-II, and **(m)** Fe6-II to Fe1-IV.

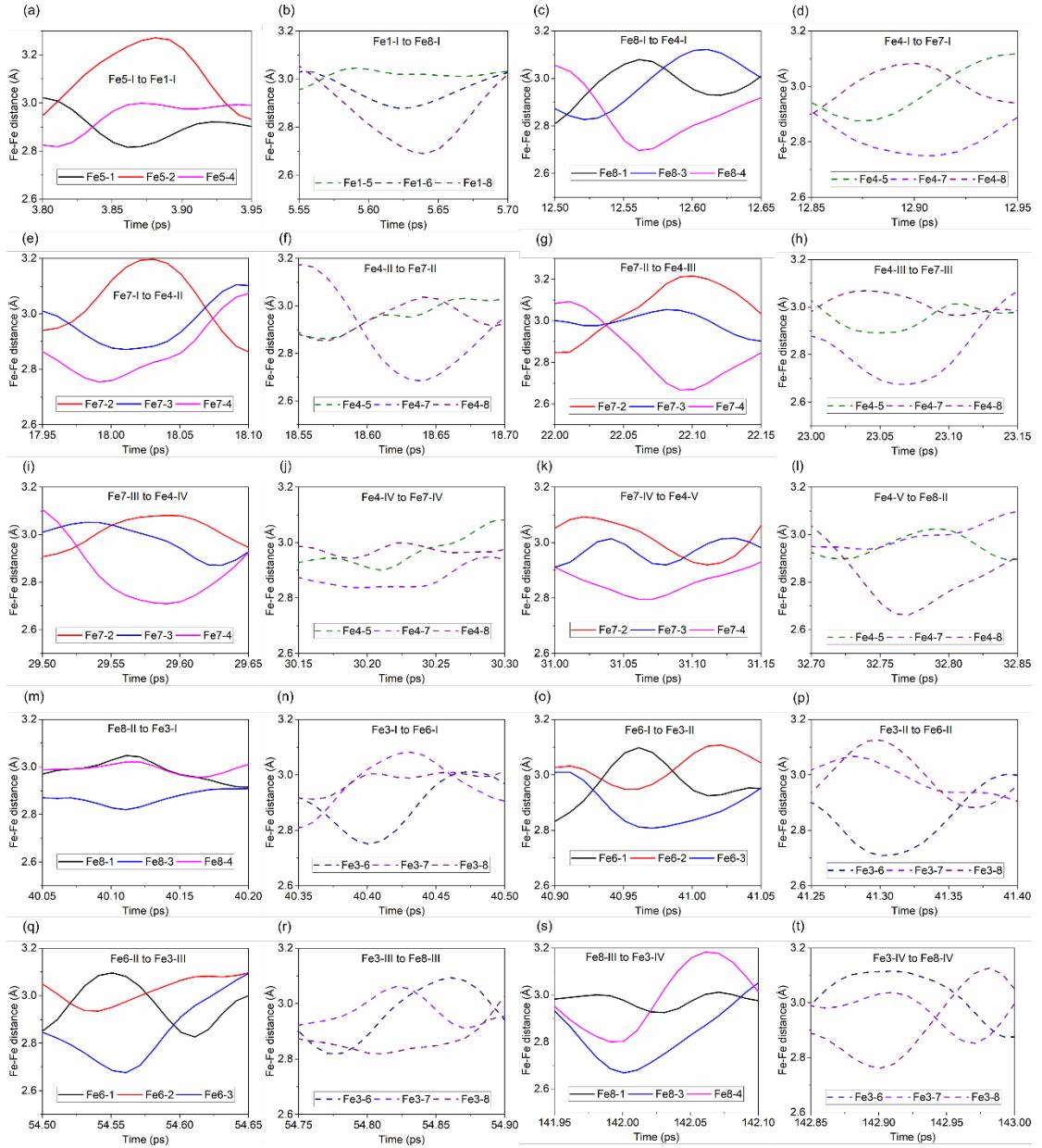


Figure S11. Three shortest Fe-Fe distances in the temporal windows of 0.1-0.15 ps for each EP hopping in Si@EP Fe_2O_3 , extracted from the AIMD trajectory of 150 ps: (a) Fe5-I to Fe1-I, (b) Fe1-I to Fe8-I, (c) Fe8-I to Fe4-I, (d) Fe4-I to Fe7-I, (e) Fe7-I to Fe4-II, (f) Fe4-II to Fe7-II, (g) Fe7-II to Fe4-III, (h) Fe4-III to Fe7-III, (i) Fe7-III to Fe4-IV, (j) Fe4-IV to Fe7-IV, (k) Fe7-IV to Fe4-V, (l) Fe4-V to Fe8-II, (m) Fe8-II to Fe3-I, (n) Fe3-I to Fe6-I, (o) Fe6-I to Fe3-II, (p) Fe3-II to Fe6-II, (q) Fe6-II to Fe3-III, (r) Fe3-III to Fe8-III, (s) Fe8-III to Fe3-IV, and (t) Fe3-IV to Fe8-IV.

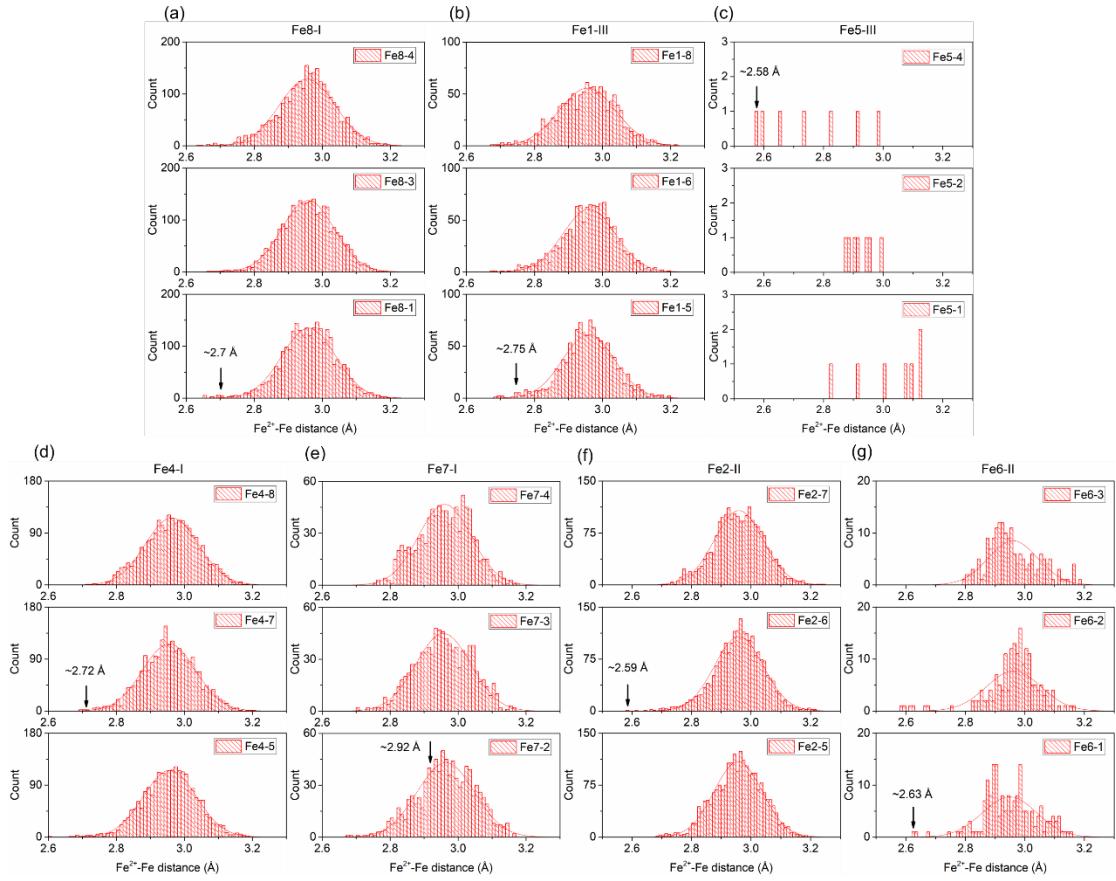


Figure S12. Probability distributions of the three neighboring Fe^{2+} -Fe distances for the stages defined in Figure 2 in the last 100 ps of the AIMD simulation on e@EP Fe_2O_3 : (a) Fe8-I, (b) Fe1-III, (c) Fe5-III, (d) Fe4-I, (e) Fe7-I, (f) Fe2-II, and (g) Fe6-II. The arrow indicates the Fe^{2+} -Fe distance around which the EP hopping takes place.

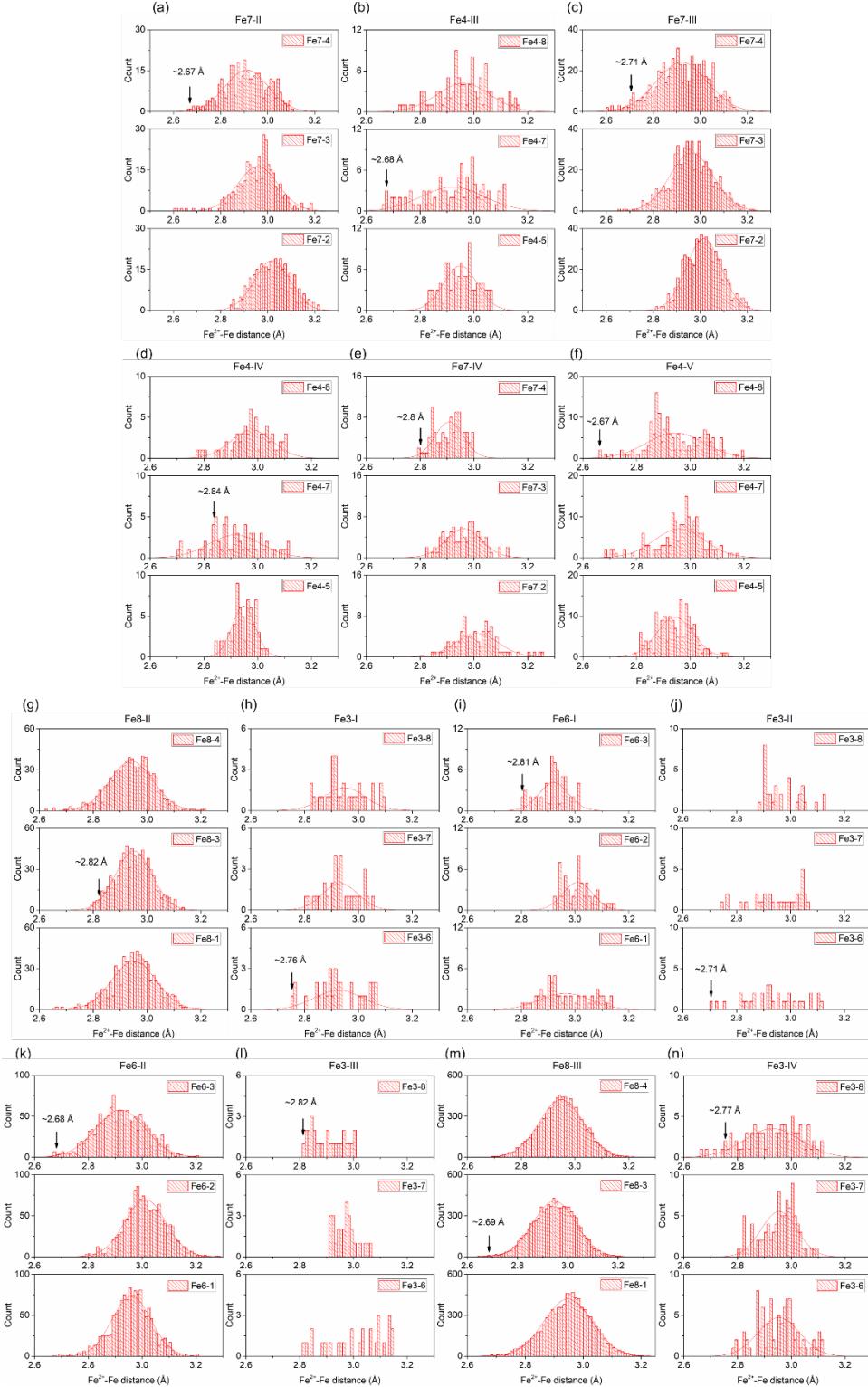


Figure S13. Probability distributions of the three neighboring $\text{Fe}^{2+}\text{-Fe}$ distances for the stages defined in Figure 6 in the last 130 ps of the AIMD simulation on Si@EP Fe_2O_3 : (a) Fe7-II, (b) Fe4-III, (c) Fe7-III, (d) Fe4-IV, (e) Fe7-IV, (f) Fe4-V, (g) Fe8-II, (h) Fe3-I, (i) Fe6-I, (j) Fe3-II, (k) Fe6-II, (l) Fe3-III, (m) Fe8-III, and (n) Fe3-IV. The arrow indicates the $\text{Fe}^{2+}\text{-Fe}$ distance around which the EP hopping takes place.

The atomic coordinates (in the format of POSCAR as the input file of VASP) of geometries used for computing charge distributions and potential energy curves.

The energies are given in parentheses.

(1) e@EP-Fe₂O₃

(1.1) 2×2×1 supercell with the EP localized on Fe1 (-823.203 eV)

10.1413002014000000	0.0000000000000000	0.0000000000000000
-5.0706501007000000	8.7826236017999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.9027004242000007
O Fe		
72 48		
0.1899439046058910	0.0164144372966085	0.0818431439837964
0.3335062666053893	0.3204762111418739	0.0831403660593800
0.4894133574279440	0.1677762272584277	0.0832779546275266
0.6806733155939675	0.0132583774239054	0.0834933847622376
0.8322708396580472	0.3223620801729066	0.0830067663784279
0.9850719987599056	0.1764169380619916	0.0812548733262581
0.1805217057316611	0.5152155564982562	0.0830553308466757
0.3350419047740289	0.8202918576301451	0.0833021064994210
0.4860096666799890	0.6658700653526853	0.0833189522414184
0.6793867674248375	0.5124762032867517	0.0833595771507631
0.8289129604530396	0.8143949701540100	0.0831270662543499
0.9871780416946722	0.6674141612482662	0.0836771929910677
0.1532052803850575	0.1534126222283962	0.2504976012644073
0.0003457513812870	0.3472041644216941	0.2503408824636767
0.3471297619500666	0.9998139161487460	0.2505216150159085
0.6533431473623231	0.1529491068146111	0.2497661978784309
0.4989682684090433	0.3458831696537781	0.2497937954951331
0.8424845486065276	0.0010639443819254	0.2548004962599445
0.1533711436752467	0.6525094178892676	0.2504271299141675
0.9982596957466023	0.8408421989367864	0.2542076564637967
0.3467569844364021	0.4999624197352083	0.2502973516182583
0.6525634279415974	0.6524973793542602	0.2506144188606859
0.4992249980477236	0.8463563650475691	0.2505639614755931
0.8467452436050867	0.4996438366950640	0.2501755374046456
0.0140251128347500	0.1798651222755045	0.4170194860830114
0.3201283763857782	0.3335526476962701	0.4171470846975747
0.1665080279751714	0.4862698040450954	0.4171483988624588
0.5134529293932533	0.1802825535200400	0.4167411803120052
0.8195124261423196	0.3328314323234672	0.4167507889144179
0.6666253165253250	0.4862187629947582	0.4167184112463326
0.0138246926629454	0.6786374338122494	0.4183135079018533
0.3201617152893043	0.8333972264382589	0.4173203088663170

0.1663495417968014	0.9861438879947083	0.4170127347179806
0.5129601821463716	0.6793115677677590	0.4173498729881160
0.8191613050592209	0.8330195534258512	0.4177037051606723
0.6648446548946226	0.9859157295618227	0.4184041228132442
0.4864845237079293	0.3197138304400657	0.5832932694604015
0.1802976293538210	0.1666848607624485	0.5835903410411254
0.3333350104017121	0.0135874971891523	0.5834038459105202
0.9863775054300969	0.3196896877307300	0.5833184883979168
0.6802567343766405	0.1668150029784289	0.5834358458241831
0.8334163215138936	0.0136152425005461	0.5836463555225889
0.4863938270983269	0.8194990338108942	0.5837449244963533
0.1804015417334434	0.6667961181958805	0.5836080300717823
0.3331529223684455	0.5132804418716251	0.5834891013531507
0.9864131922484848	0.8197610495207418	0.5836476623959682
0.6802180164626139	0.6665195029094733	0.5836009868961211
0.8330355032578354	0.5133112554679524	0.5834379085584168
0.3467846067806871	0.3468698308681377	0.7497796329101286
0.1532026012537079	0.0000966708699962	0.7499809564525477
-0.0000572214564890	0.1530688381996236	0.7498777890398441
0.8467624504703397	0.3471530816274803	0.7494975016261761
0.6533346308404551	0.9998522342357068	0.7498082083047628
0.5003397116942178	0.1532973426085145	0.7495761734051503
0.3471119611858841	0.8470101429947109	0.7496541146616612
0.1531454221673451	0.5001380967481236	0.7494184297417852
0.0003353161503291	0.6535868391591837	0.7497398874592730
0.8470192053928409	0.8468658602001672	0.7500482334328894
0.6530164463686530	0.4998355624603482	0.7496885801094179
0.5001890941307631	0.6531666556089004	0.7497613716313565
0.3200962880154594	0.4872945582948032	0.9160375778652285
0.1667443608360705	0.1806473733008742	0.9163807027468112
0.0139888272721541	0.3347330945285285	0.9149213244626092
0.8200041533235876	0.4874079248697875	0.9160530034991460
0.6670868694960653	0.1806138767863224	0.9160442129573680
0.5135463900453521	0.3333231524504315	0.9161277557905055
0.3206364536108557	0.9863844026942370	0.9154090853150204
0.1672428508437226	0.6805514084708856	0.9161700049879807
0.0140094692153359	0.8336925708713103	0.9168333964008204
0.8198543391937330	0.9866274728107393	0.9166931645256354
0.6665501488764003	0.6800241461248112	0.9159998942593742
0.5136244543487564	0.8332193889487771	0.9163104960970948
0.1666765447555744	0.3341128374527715	0.0207274668142418
0.6666052334905126	0.3338310596043802	0.0205302738087794
0.1680786154746080	0.8350095863015787	0.0216191906162654
0.6667848892729212	0.8328906935925159	0.0211640369783529

0.9957640368354621	0.9995373052196103	0.1447935017914002
0.5015469403439120	0.0015648457344164	0.1462580220739214
0.9989125384674146	0.4993638286492303	0.1458951850421857
0.5002612496996373	0.4990923401850321	0.1461599072154771
0.3296393506774641	0.1635437527471403	0.1862355809959459
0.8363429389677370	0.1646091241413496	0.1867824476137812
0.3332979123950129	0.6666285453020814	0.1871658530924936
0.8347132705768275	0.6688863365887032	0.1879864527735724
0.1664604456702757	0.3323791119825190	0.312553559853221
0.6661234696168586	0.3325622754452890	0.3114261730363917
0.1667413445688286	0.8326270047339397	0.3130805339778926
0.6655225601440971	0.8327051726411848	0.3135364909523123
0.9988618886370312	0.9983274188411809	0.3511795541458743
0.5000243245984914	0.0001512324497821	0.3536977196878173
0.9997926429222099	0.4994205924570565	0.3537497255692491
0.4999465015979910	0.4995245199630325	0.3535738299406230
0.3328036760064061	0.1661963427032214	0.4790639013569381
0.8336110599246607	0.1662986008584370	0.4789573087007145
0.3331421657868016	0.6664528144315639	0.4794854221452005
0.8333099748527479	0.6665338162429650	0.4792202241665010
0.1664709916966347	0.3329852025382840	0.5202764719593340
0.6665840449657322	0.3331402127148315	0.5201330688978618
0.1664676282275734	0.8332825821405080	0.5204906152837038
0.6667680833855424	0.8333193864649220	0.5207755719704005
0.0000823896281896	0.0000474482558939	0.6463686247693340
0.5000490129921175	0.0000476242717871	0.6459945131270877
0.0000059451875158	0.5000043611280276	0.6459305280430239
0.4999004988774606	0.4998130128286007	0.6460866154942215
0.3334209812031353	0.1666668662773835	0.6872406117289873
0.8333228148688353	0.1667762226012397	0.6872034523475867
0.3335234255336761	0.6667730176001405	0.6872642785275319
0.8333012986912227	0.6666479700571163	0.6873018117962840
0.1664769155029883	0.3335973071702046	0.8128233224490857
0.6667515952728403	0.3334261959732956	0.8130299819078771
0.1672599643001001	0.8337587417772716	0.8131768048770034
0.6668375841415565	0.8331400329906561	0.8131436639701413
0.0001005816397773	0.0001690966518672	0.8547518438564170
0.5009609851375112	0.0002808728252048	0.8538660720961726
0.0000946564654394	0.5010941102053000	0.8537210070089634
0.4997887702634140	0.4996281355770961	0.8540654380728575
0.3329526108323675	0.1654788041581841	0.9796964155352772
0.8350473348986733	0.1687708302601669	0.9797166369556424
0.3333799413853303	0.6670179255511901	0.9794946513017462
0.8332533795472329	0.6671993129125842	0.9802325082581211

(1.2) $2\times2\times1$ supercell with the EP localized on Fe2 (-823.203 eV)

0.1795459540506797	0.0129665938141586	0.0831790222721628
0.3321153181831390	0.3216025984549323	0.0833486562930136
0.4834716875592507	0.1735524744010640	0.0819449540527320
0.6854201373848477	0.0141820823694550	0.0830970462940603
0.8325818164907608	0.3196527594366551	0.0837464984032705
0.9874100399591464	0.1668336263185195	0.0833964119551720
0.1775765430235882	0.5098979110170390	0.0829636239041104
0.3237695547201172	0.8086517825867995	0.0811095805008463
0.4867376448858776	0.6672589440543325	0.0834891751355277
0.6797459977364881	0.5146976524161410	0.0833885701762958
0.8341522840550755	0.8200715546007350	0.0833498084851720
0.9847107217314534	0.6652505858782020	0.0830506706209941
0.1540616976584174	0.1531725023219622	0.2498656520687264
0.0004118642956411	0.3471811677951376	0.2501936926791734
0.3466907031999070	0.0000420778846190	0.2505399481833203
0.6592696165390468	0.1576292405515571	0.2542182216582524
0.5001916674716753	0.3474451736345539	0.2506011958074755
0.8475749650504527	0.0001435995180412	0.2506576299600959
0.1528026334796925	0.6531652406920102	0.2502975094231011
0.0001021599751137	0.8468522996993331	0.2502812591879581
0.3470969235823519	0.5004928256509426	0.2497808555347136
0.6536631263070465	0.6529259640053922	0.2505615240701426
0.4990851718105301	0.8415948921059462	0.2547596198014463
0.8475586626499965	0.5009744032373390	0.2505075421561209
0.0138268619313706	0.1805653074655468	0.4167258134709061
0.3197584117194223	0.3333029984009279	0.4167841778702457
0.1672062342904438	0.4868381980397496	0.4167363655971366
0.5139358522091479	0.1803528273052988	0.4170715308581622
0.8214103467846099	0.3352988137102147	0.4183417402173694
0.6666253984090942	0.4868729017167203	0.4174102722703840
0.0138481505970637	0.6804232672503577	0.4171477868386336
0.3201930409357198	0.8342309701672367	0.4170242520049507
0.1665958399955560	0.9867492515636177	0.4171699261525402
0.5141952693717456	0.6791170022261646	0.4184388565548884
0.8207547287478476	0.8337740104237673	0.4173812567722070
0.6671389296835492	0.9863477235891326	0.4176928090703779
0.4864153422098689	0.3197557132496052	0.5834428414534781
0.1802781582795140	0.1667846724115747	0.5832893130944629
0.3333784055207735	0.0136720796545929	0.5835867636692450
0.9866977270249365	0.3197812689096082	0.5834597173903358
0.6802215076245415	0.1667097336476813	0.5836935122996405
0.8335121881691074	0.0137519722467789	0.5836262899828061

0.4863972222903146	0.8198580300797654	0.5836592035412962
0.1803283273615479	0.6667540550376008	0.5832803762879978
0.3332037158631643	0.5134995602170945	0.5834365292934011
0.9867516783722008	0.8198951129171699	0.5834933604294871
0.6805117746058658	0.6669317771556731	0.5837918033832358
0.8331758188304553	0.5136497109392784	0.5836520879767192
0.3466899077372969	0.3469777994198339	0.7495841557687578
0.1531193561633790	-0.0001811280061851	0.7497985344844430
0.0001216700079002	0.1530775070865186	0.7497060750536104
0.8463233326520493	0.3466485982872483	0.7498064712116660
0.6531183592005487	0.0000927304994964	0.7500848810379900
0.4998286494559788	0.1530036082860340	0.7500527537664599
0.3468691445071756	0.8467729993353100	0.7498761310079923
0.1527943399057053	0.4995217731014157	0.7494927007926626
-0.0001951115196598	0.6528994116609382	0.7494365836134490
0.8468218241724440	0.8469789605278698	0.7497653401864866
0.6529321659797369	0.4999720453042049	0.7497219939051222
0.5001306622294586	0.6534106374852645	0.7497871905805790
0.3192627531355152	0.4862936721072069	0.9160194201454115
0.1665453786794727	0.1800680945014932	0.9161757328498918
0.0125059837987496	0.3324776876097823	0.9160493811726712
0.8193789708009591	0.4864930972633833	0.9162737504729214
0.6661452146012422	0.1800760327759093	0.9169432548986283
0.5135739395050932	0.3342171707108295	0.9154691232272097
0.3192797134583777	0.9859797160637774	0.9163956184264263
0.1652201109137609	0.6791290601475621	0.9148648611445135
0.0126861458032332	0.8326402719479837	0.9160246831761033
0.8199566008332647	0.9863792791245740	0.9160229105373938
0.6667892981433199	0.6802812085513964	0.9163170223594652
0.5133507587661924	0.8330885616165559	0.9166549902069697
0.1660942620386500	0.3326984939300468	0.0205441250667667
0.6650518278781912	0.3330454977798866	0.0217039623632539
0.1658699848146725	0.8324814531513585	0.0206976862119048
0.6671097402037679	0.8337157761297799	0.0211085449465001
0.0008755755427146	0.0010653558802755	0.1461529655901155
0.5005540735135838	-0.0036031463619514	0.1448247039150745
0.0007219307098159	0.4995958026303235	0.1459104003611944
0.4984181113422448	0.4999982886903614	0.1463020708114723
0.3363742628222374	0.1662830600020117	0.1863267778701261
0.8311521696727618	0.1659029735914566	0.1880414370941579
0.3354528114750197	0.6718727501858686	0.1867099317881476
0.8333920051923661	0.6666478558773927	0.1872073119365186
0.1674490094888665	0.3337161195299598	0.3114921877404062
0.6673466151400952	0.3342288870034483	0.3131754016199783

0.1676907641375556	0.8341610754717386	0.3125378032201558
0.6674226324055872	0.8329354237708556	0.3135485762535850
0.0005283535362573	0.0005173860075840	0.3536002776104014
0.501727374828946	0.0006331003606054	0.3512054233968023
0.0005538932739447	0.5004611006264749	0.3537616597386800
0.4998636536607104	0.4999993035584500	0.3537403191476711
0.3339071193874972	0.1667376412999608	0.4790641443073122
0.8335195635134279	0.1669442741986872	0.4792624140300683
0.3337219615492010	0.6674390368612860	0.4789527078791336
0.8336374709318061	0.6668313638762535	0.4795136454046224
0.1668696174104475	0.3335107555233279	0.5201401692763616
0.6667375733523584	0.3332309532080662	0.5205588133273219
0.1670488665119504	0.8336144305977792	0.5202877657366693
0.6667204458306477	0.8335464201791151	0.5208252780588257
0.0002049774090893	0.0000908607873348	0.6460618927961130
0.4999587475432061	0.0000566811555104	0.6464030844838820
0.0000091278970430	0.5000317609270919	0.6459512244933737
0.4999400021177360	0.5000092302333726	0.6460209630518562
0.3332674964218123	0.1666514006671312	0.6872711174337968
0.8333467555165482	0.1666528414238038	0.6873543700021463
0.3331843587910526	0.6664726496113830	0.6871968001795384
0.8331787105303768	0.6666649849080745	0.6872976024866878
0.1665491720122536	0.3332018396829562	0.8130061953214023
0.6661394027264063	0.3333447094502760	0.8132609175107350
0.1663743227126957	0.8327242674290043	0.8128336435467763
0.6668507150567854	0.8336147287331493	0.8131251548930170
0.0002805214219926	0.0000303330695172	0.8540702756911482
0.4997283013068499	-0.0002285779590672	0.8547875846108931
-0.0011674585727548	0.4988287855871795	0.8537546980446024
0.4996949874951968	0.5005291350935406	0.8539224766071756
0.3343891854077856	0.1673442607798324	0.9797584585738305
0.8327092856055195	0.1658960705503782	0.9802864359554816
0.3312258628783504	0.6661871462521930	0.9796142389171832
0.8329666899974602	0.6662315798785281	0.9795597475665576

(1.3) 2×2×1 supercell with the EP localized on Fe3 (-823.203 eV)

0.1797468872428310	0.0147398649783258	0.0833205818239122
0.3342276003595253	0.3201029231404598	0.0832817841708414
0.4847644355574410	0.1652438615250425	0.0830174258409209
0.6776172782235478	0.0099356097805923	0.0829742697460311
0.8237305112149869	0.3086698922211249	0.0811685512609788
0.9867471871787996	0.1673537536770548	0.0834447188837810
0.1855025635868567	0.5143182228928651	0.0830690299539281
0.3326338075920828	0.8196848493033481	0.0836796800488668

0.4874779030012787	0.6668402116096603	0.0833689242072844
0.6796070355656582	0.5130505406555121	0.0831666666854601
0.8321436625046750	0.8216500946059963	0.0833539904629961
0.9835622034571038	0.6736211338816926	0.0819429278251431
0.1536489730637689	0.1528653622537633	0.2505327845714084
-0.0010225050147472	0.3415254138907922	0.2547660211680030
0.3475591067516964	0.0009661108271324	0.2504690218121064
0.6527814874440601	0.1531886485510711	0.2503193073818540
0.4999629845951470	0.3467910136078200	0.2503161304909376
0.8470612331378647	0.0004941039581240	0.2497609968033530
0.1591669762757376	0.6575723124795110	0.2541560973522708
0.0001466098599676	0.8474048911361975	0.2506013850865484
0.3474859228448770	0.5000826834136407	0.2506244273489394
0.6540595293958338	0.6531304180107045	0.2498279334191011
0.5003746327865383	0.8471539253010721	0.2501668494169277
0.8466206451563719	0.4998933541282444	0.2504898867092427
0.0140441028725417	0.1790136293570696	0.4183766999423377
0.3206067055894101	0.3336621734171030	0.4173398668348841
0.1670106120272896	0.4862381295612971	0.4176773157278654
0.5137409664405331	0.1803211171121965	0.4171518428831895
0.8200721214494885	0.3341862011145113	0.4170445184388126
0.6664488917560033	0.4866577639639142	0.4171582973659666
0.0138475484349103	0.6802886549850433	0.4170530545229298
0.3213307290644374	0.8352281765496398	0.4183037354453698
0.1665710051111634	0.9868033377133186	0.4173557047718729
0.5137515776841133	0.6805253818779324	0.4167132894339140
0.8196267081178720	0.8331806239974423	0.4167492929176670
0.6671648131204915	0.9867277453198571	0.4167425154796250
0.4866981431921614	0.3198886668600991	0.5834802899681525
0.1804263709706831	0.1668488870157504	0.5837288775038878
0.3332110082563631	0.0136119395442473	0.5836200769253027
0.9863165255376262	0.3197794076617572	0.5836170879122209
0.6802875993883549	0.1667001018799214	0.5832880948864665
0.8331586530611594	0.0134496139994740	0.5834347841503158
0.4866692225665622	0.8197240465186436	0.5834634239607933
0.1802375999450541	0.6666567015655602	0.5836450537509359
0.3334750566315971	0.5136789647466047	0.5835594945104609
0.9864019154334530	0.8197652754905912	0.5834062443243648
0.6802764266396913	0.6667877353180017	0.5833066318016779
0.8333430650099574	0.5136630986689598	0.5835800452165846
0.3468319393383318	0.3469932551785725	0.7497451376415120
0.1529919398035921	0.0000045240298624	0.7496824627338117
0.0001223556841765	0.1534483913155237	0.7497803800552293
0.8469333182437785	0.3468517930766960	0.7498706530669061

0.6528412897712472	-0.0004123007508485	0.7495002594549527
0.4998808994651772	0.1529887792240197	0.7494396014881812
0.3463961566977695	0.8466473836805204	0.7497639809062415
0.1531339725987214	0.5000897989214713	0.7500343124057018
-0.0000777839739022	0.6530538270070554	0.7500052406007471
0.8467490505106621	0.8470243462686584	0.7495895194084087
0.6532011941541402	0.4999079068377730	0.7497895029250364
0.5001529240598881	0.6531148254901737	0.7496895471392290
0.3200199260372127	0.4864431117226852	0.9159919898737833
0.1668580819146545	0.1803118275066730	0.9162695274269256
0.0134851540059410	0.3331739667211300	0.9166213689609287
0.8193550525463298	0.4860228378194120	0.9163908400902357
0.6652915823580815	0.1791992504785376	0.9148824699596166
0.5127595137915677	0.3327532422831686	0.9160199157978824
0.3194787666405577	0.9865881802433720	0.9162049182464703
0.1662425080291434	0.6802183729084803	0.9168857055903006
0.0136236639235431	0.8342277647889409	0.9154398377964276
0.8194020543749391	0.9863986087366847	0.9160323252012657
0.6666373619006339	0.6801390450879371	0.9161527268775699
0.5125959515154958	0.8325557595487267	0.9160513235862988
0.1671829728898846	0.3337938863300724	0.0210922436146377
0.6659063888364843	0.3325312512262782	0.0207166445632584
0.1650660658135286	0.8330864001593530	0.0216502139848426
0.6661525991369054	0.8327833292898079	0.0205412253703163
-0.0015664462236770	0.0000438697701810	0.1462601258775745
0.5006972565992642	-0.0004488416393901	0.1458847106526487
0.0005433733298010	0.4963907067339750	0.1447469855220613
0.5008985130770796	0.5011094278322721	0.1461457172841884
0.3333912346534105	0.1666463302906354	0.1871532665468219
0.8353781386417296	0.1718348118040631	0.1867412562086300
0.3311295262995797	0.6658652944468071	0.1880180711950574
0.8363909502258097	0.6662078181079493	0.1863216088968247
0.1672935508860320	0.3328205893023448	0.3135011913063515
0.6675999133671408	0.3341386894957338	0.3125392789908417
0.1673646519695604	0.8342135774595891	0.3131157596792219
0.6674406558310253	0.8336672015109533	0.3114521711814183
-0.0002373773904874	-0.0001228643308860	0.3537127807473963
0.5005838728900019	0.0004291147633346	0.3537485854958735
0.0016448761630731	0.5005842874108162	0.3511540199195252
0.5004260477899224	0.5005042167473441	0.3535891811933774
0.3335435116485947	0.1667478984434855	0.4794949766086815
0.8336708043362374	0.1673772686125502	0.4789407495094353
0.3334064494512994	0.6668425720268647	0.4792344420179998
0.8337698657517852	0.6666114950454028	0.4790718818130096

0.1666541885910692	0.3334674123456372	0.5207566478241772
0.6669872712981527	0.3335239650071000	0.5202874896805738
0.1666879931343134	0.8331900042780312	0.5205145746234110
0.6668142273640664	0.8334521371964049	0.5201499642715169
-0.0000919267148711	-0.0000183490893434	0.6459897743194407
0.5000137437973527	-0.0000027359773960	0.6459420177772459
-0.0000473013659150	0.5000314931787748	0.6463768025278903
0.5001799309695303	0.5001057526610457	0.6460589852613524
0.3332235643422432	0.1666982994368869	0.6872789894712144
0.8332318347336447	0.1665425841584620	0.6871922013207560
0.3333468590368938	0.6666348963588666	0.6873092797022813
0.8333411909061542	0.6666916669763676	0.6872644279115240
0.1668810146173883	0.3336525314726532	0.8131020146438799
0.6664597602604581	0.3328452502404182	0.8128330257544515
0.1662483843323919	0.8334071901126668	0.8132082556094011
0.6665982138139158	0.8332630517820915	0.8130248198432469
-0.0002343372891080	0.0005746789068153	0.8538731513211008
0.4989544522840618	-0.0010447490483872	0.8537273633696149
-0.0001729527875944	0.4998547332360803	0.8547703932713450
0.5003712423587257	0.5001159376988672	0.8540406044954434
0.3330481564424200	0.1662890028860289	0.9795013630870072
0.8313374868102362	0.1662738263751336	0.9796509946673490
0.3327885157345338	0.6659652392383090	0.9802600252819237
0.8344700078814771	0.6674166075350579	0.9797586604037937

(1.4) 2×2×1 supercell with the EP localized on Fe4 (-823.203 eV)

0.1775296638988950	0.0098864594904548	0.0828756767353683
0.3237655789899154	0.3086449919922368	0.0810497242043729
0.4867062314112072	0.1672482587193708	0.0834417002043438
0.6797044910517636	0.0146507356987682	0.0833828900821327
0.8341416689254200	0.3200373828950028	0.0833142708917892
0.9846867444401258	0.1652156433799164	0.0829975223989163
0.1795423752553227	0.5129228529914100	0.0831521626640514
0.3320915512990337	0.8215750834534763	0.0833208442786446
0.4834659313677361	0.6735489851535839	0.0819554139040291
0.6853848919500241	0.5141544765727362	0.0831011367232782
0.8325490271359929	0.8196104327404483	0.0837648817504069
0.9873586119486656	0.6667772493935004	0.0833941155018580
0.1528792971052447	0.1532647710212051	0.2502385520357527
0.0001361795970754	0.3469022916067299	0.2502199740925874
0.3471338494210391	0.0005587663780779	0.2497244969112869
0.6537020262266630	0.1529650165925935	0.2505471755176473
0.4991485772838358	0.3415963690244834	0.2548001824126955
0.8476218552150809	0.0010533605042919	0.2505017298924438

0.1541145589922263	0.6532367611675850	0.2498293369883546
0.0004659752327347	0.8472443708833877	0.2501553048215922
0.3467433995666365	0.5000738319695621	0.2505474682227289
0.6592869786614727	0.6577158945093013	0.2542094907475846
0.500228521719964	0.8474922673814852	0.2506089449092809
0.8476447881799641	0.5001921596368938	0.2506614457647094
0.0139205600202965	0.1805537760587902	0.4170988183346432
0.3202558961142006	0.3343232803751154	0.4170228118099049
0.1666842970689719	0.4868828698125789	0.4171130697216024
0.5142729399263259	0.1791930494011667	0.4184359997614897
0.8208486385723802	0.3338833547886313	0.4173624923659987
0.6672361444277169	0.4864531115360849	0.4177113416213291
0.0139005388164459	0.6806893680596120	0.4166865421384994
0.3198209623926332	0.8334069829456145	0.4167552540120243
0.1672971522429923	0.9869459534100010	0.4166789610094079
0.5140272588903079	0.6804387216940385	0.4170819112932807
0.8214974693792164	0.8354196535063761	0.4183348324345986
0.6666789652926567	0.9869616537647450	0.4173988793156193
0.4864310097457898	0.3198891938207646	0.5836376979246298
0.1803202981534713	0.1667735899863389	0.5832481665860684
0.3332134000390389	0.0135332658421483	0.5834132026133083
0.9867718255044793	0.3199340831387514	0.5834537266333528
0.6805250670662757	0.1669609542558444	0.5837754569707568
0.8332267642033445	0.0137074080913919	0.5836236653463857
0.4864270776793146	0.8197909909408917	0.5834418813276129
0.1803025733414644	0.6668407349785960	0.5832618950710048
0.3334093800484682	0.5137296429258104	0.5835630520175921
0.9867337392995433	0.8198119721166992	0.5834483519124116
0.6802673525505322	0.6667705475794102	0.5837095452847549
0.8335580150881333	0.5138255744615566	0.5836177222330934
0.3467987720616228	0.3467060861725801	0.7498225915668363
0.1527474486570918	-0.0005431710728039	0.7494708033881753
-0.0002560753084692	0.1528139315218612	0.7493983429406718
0.8467706731534216	0.3469128887600286	0.7497277543877467
0.6528942567479223	-0.0000974879837472	0.7497082578780206
0.5000594209397866	0.1533265034044905	0.7497605181405430
0.3466551202293647	0.8469067308033401	0.7495717193305694
0.1530683119156481	0.4997688924859817	0.7497495016539822
0.0000560544531341	0.6529826717742016	0.7497121288580944
0.8462763173851079	0.8465800080564854	0.7498078043120295
0.6530772955800839	0.5000119901309723	0.7500601033695350
0.4997845323492358	0.6529354100369910	0.7500398624858584
0.3192117162197118	0.4859021570113096	0.9163650252358452
0.1651721055526004	0.1790650694685648	0.9148164943896260

0.0125867552246470	0.3325246306424404	0.9159744464420804
0.8198782709104875	0.4862877048420708	0.9160188556483588
0.6667076596266865	0.1801814417126341	0.9162857452775538
0.5132926104252787	0.3330014424202091	0.9166008889016891
0.3191919445257074	0.9862069689406185	0.9159683919218028
0.1664602115938064	0.6799566929977154	0.9161692079887770
0.0124056449156965	0.8323422885269557	0.9160262775081687
0.8193150413586877	0.9863633455343671	0.9162751094278396
0.6660209802785088	0.6799535528698977	0.9169612669398175
0.5135116690824880	0.8341256034681285	0.9154734765860518
0.1658613387780607	0.3324253209601774	0.0206408150735755
0.6671008119136995	0.3336931574921195	0.0210839890381484
0.1660011491376315	0.8326176500164478	0.0205097397101421
0.6650121435347204	0.8329662476581986	0.0217139638821349
0.0007255344138573	-0.0003982207279100	0.1458685292212673
0.4984103658551758	0.0000012884012070	0.1462637113840655
0.0008965475889059	0.5010443652462268	0.1461210185183964
0.5004678184311419	0.4963628397954032	0.1448408184772301
0.3355250975229344	0.1719380382540623	0.1866857791769887
0.8334016379932808	0.1666736371503254	0.1871765450643681
0.3364129753582219	0.6663314985143760	0.1863168929820630
0.8311514842868845	0.6659029296524336	0.1880434909416791
0.1677468494337253	0.3342376406521909	0.3124984467130730
0.6675116787348937	0.3329740891353585	0.3135659577516050
0.1675166167168471	0.8338068924952748	0.3114477422137347
0.6674292569975158	0.8343113565719164	0.3131796530508686
0.0006518230294153	0.0005922125459739	0.3537081125819618
0.4999530551587240	0.0000930291573783	0.3537086167300447
0.0006275410552356	0.5006528064440082	0.3535606797177064
0.5018529525503587	0.5007339325229684	0.3512350424245297
0.3337931276624126	0.1675142623408463	0.4789247879906160
0.8337104418571557	0.1669269940088066	0.4794718391529229
0.3339570214894712	0.6668478707743578	0.4790513362604233
0.8336153708549686	0.6670775601737631	0.4792613949473643
0.1671159726086883	0.3336894504866775	0.5202500778434559
0.6667875980951681	0.3336323032634859	0.5208337791220042
0.1668947176160828	0.8335670420349146	0.5200942366772657
0.6667714498586370	0.8333032266435788	0.5205800475749099
0.0000097631618688	0.0000422257116815	0.6459223868329012
0.4999390031365915	0.0000263768424713	0.6459973324358805
0.0002308008321663	0.5001029500990144	0.6460280147125723
0.4999693463304537	0.5000645874411851	0.6463751552508293
0.3331355202075558	0.1664159313585710	0.6871669689467332
0.8331065435251372	0.1666074343043052	0.6872732068786471

0.3332458045117614	0.6666181302590317	0.6872572126401315
0.8333110929339359	0.6666025555827786	0.6873615556322887
0.1662774574911925	0.3326399350664311	0.8127695584683217
0.6667842309186296	0.3335152724278619	0.8130914676261249
0.1664865289154772	0.8331218193225558	0.8129802157728003
0.6660807384389682	0.8332598137252860	0.8132739493633726
-0.0012399719726091	-0.0012762328088864	0.8537335480056757
0.4996265554645943	0.0004122072708792	0.8538943488150317
0.0001889714992081	0.4999111558555656	0.8540467979969809
0.4996436641813404	0.4996675323490507	0.8547484041180669
0.3311683005899825	0.1660942928734377	0.9795771768475786
0.8328920031905034	0.1661190061694215	0.9795323169220234
0.3343067467317206	0.6672475136796856	0.9797520078929414
0.8325931793074005	0.6657843976323746	0.9802951296436833

(1.5) 2×2×1 supercell with the EP localized on Fe5 (-823.203 eV)

0.1799716661305856	0.0132731111377156	0.0828007687726189
0.3348785804450521	0.3258438193510401	0.0791522773875764
0.4908750404109400	0.1657108688485535	0.0785785417464477
0.6798654746762419	0.0137569355045823	0.0835706634827674
0.8340925781555830	0.3203341311861355	0.0827972069254225
0.9860631298278936	0.1668069193950552	0.0827181721092033
0.1799037743070672	0.5142545913814115	0.0828310700038620
0.3329148914750120	0.8194858989470534	0.0830659800426808
0.4865540508182298	0.6670752623653851	0.0831817114571998
0.6807386724272932	0.5141657840835591	0.0826931954219957
0.8342357760625007	0.8207508680270541	0.0835192506266905
0.9865383202470295	0.6666975918199471	0.0830326809532644
0.1432591708985081	0.1502446403420433	0.2513805447233722
-0.0016442875334252	0.3463760950945879	0.2499777153853667
0.3483898339192439	0.9904120820698674	0.2522251570021672
0.6527333484167462	0.1533794239577062	0.2499279091155206
0.5045696585602112	0.3521745736487378	0.2502829217194559
0.8438322841670721	-0.0012365715835610	0.2499602104730684
0.1528845123072632	0.6514149691018909	0.2503376176109005
-0.0000853108248060	0.8462764027537802	0.2501830334032661
0.3462809062208012	0.4992662634922903	0.2496059927118702
0.6539694517055246	0.6541186089783964	0.2499451085041613
0.5009609315930168	0.8442796775033903	0.2504149467485430
0.8474667060231700	0.5008831740817583	0.2500435516376472
0.0127160574256171	0.1802354537721678	0.4178519687498740
0.3193517901802521	0.3328186515155689	0.4164130436567192
0.1662801920903808	0.4861056378742415	0.4170942742756387
0.5136819829412396	0.1801151535539677	0.4167445416943552

0.8199247369855677	0.3334996007817888	0.4170641916557348
0.6669416491311395	0.4866446611786432	0.4173304069903779
0.0133729991538609	0.6793912493263425	0.4173291939173658
0.3194654471828406	0.8319438550625639	0.4184725892976187
0.1666642012675200	0.9859735899538870	0.4169489553563725
0.5133751867556219	0.6791767633502273	0.4172792840395458
0.8198437558501530	0.8332461098684342	0.4171668196345535
0.6663511455112675	0.9860084040633890	0.4173278983815827
0.4863754708642380	0.3197949893348134	0.5832857405824639
0.1802047302546284	0.1665484025768963	0.5833062956324382
0.3334224840406556	0.0135808513798983	0.5834777002706285
0.9863447276580389	0.3196400424610457	0.5836224598037251
0.6800394573110040	0.1667857512646188	0.5835715645139817
0.8330523951480068	0.0133826987308492	0.5837499689416072
0.4866017096200650	0.8194705457630407	0.5838527541985453
0.1802338267743037	0.6665059917812244	0.5839043354917400
0.3330667503477616	0.5130267777473549	0.5835572764970596
0.9866393598695042	0.8198508661377766	0.5835493968648705
0.6803825127312854	0.6668130357849397	0.5836520498700072
0.8331945091818393	0.5134967680714569	0.5835935164103214
0.3468995960907229	0.3469127877186254	0.7496658194169085
0.1530059757973285	0.0000211004791308	0.7497545024496500
-0.0000277880683417	0.1530698083998606	0.7499145856346006
0.8468986211481901	0.3470965994578034	0.7496019768285407
0.6530316171822311	-0.0001634151046913	0.7499217055367593
0.4998638332598784	0.1529870669022209	0.7497035927398343
0.3469147148631460	0.8469642562674451	0.7500678920200819
0.1529091340391635	0.4998735226531822	0.7497042297778227
0.0001525768345602	0.6533983486008654	0.7498771879659581
0.8468241783314547	0.8469432480334440	0.7500568857417523
0.6531172077424586	0.5001608230592557	0.7497569834285065
0.5002640781236458	0.6533384273065667	0.7498755014635615
0.3194007840550905	0.4880468827618502	0.9150197664759515
0.1668949105154173	0.1805725789724388	0.9162688276019948
0.0130532133211800	0.3332573030008539	0.9159505463420894
0.8202889811074000	0.4873448960360844	0.9159885329110274
0.6683334335660512	0.1807714293723042	0.9149508095677302
0.5140933706588912	0.3337346324280719	0.9156451349748240
0.3192189941135929	0.9868095713068328	0.9163071698937590
0.1667405782168549	0.6804750501115220	0.9161949033971186
0.0131377904679611	0.8331984545642226	0.9162083688183617
0.8197337434504984	0.9863265531647800	0.9165822150909341
0.6665446685264939	0.6804540033705294	0.9166247826926250
0.5137120511917533	0.8338442770359172	0.9166109902777723

0.1664533284369452	0.3340243507575678	0.0201786452283813
0.6678215931372601	0.3339978874182652	0.0198157248765807
0.1667965615739640	0.8343138600526803	0.0208096952783963
0.6670769648598021	0.8341397759275015	0.021888275423669
0.0034356703200193	0.0030497769126815	0.1469913660686817
0.4968657844945720	0.0020688496447828	0.1466282434422058
0.0000963006998726	0.5000732581824664	0.1461817140755711
0.4986116591964462	0.4977974387451381	0.1452917873814392
0.3374541822169339	0.1672343803418957	0.1885656321681564
0.8317016584490026	0.1650708405233093	0.1870670884062146
0.3344911923033786	0.6673669745767467	0.1874581656870366
0.8331772135238082	0.6675768157229993	0.1871904808924531
0.1653312867214566	0.3317414411709517	0.3116422322980704
0.6667661395313577	0.3338442268499978	0.3122678795979730
0.1667441160694176	0.8325554010574420	0.3126436754754621
0.6667065738870632	0.8327587752478672	0.3128089309467824
0.0003648692492117	0.0010722405167379	0.3535591965939246
0.4984058019145524	-0.0020361156584462	0.3537295514093773
0.0001299343153898	0.4996882672171326	0.3538390765145197
0.5001520459488793	0.4993849208941228	0.3530645624648558
0.3333140901992270	0.1664343316383954	0.4785615312413503
0.8325432656817617	0.1664059012652519	0.4794551061133254
0.3333643537323379	0.6655572424264247	0.4796023361267055
0.8336207638864643	0.6670153725287946	0.4792990859153017
0.1661789577624963	0.3328634161381144	0.5200863492987715
0.6665815021370077	0.3335284239218443	0.5202484239496692
0.1669798107479412	0.8331017205558154	0.5205169930022896
0.6667087650429533	0.8332589847563081	0.5203175485465340
-0.0000149432438960	-0.0000058823002184	0.6460646791995808
0.5000316587622675	-0.0001165682676823	0.6461601078142327
-0.0001529786998937	0.4998589989697137	0.6460522246203043
0.5000568623278028	0.5000081381657319	0.6460052862596591
0.3332531034623312	0.1666090539046626	0.6869418359648607
0.8332331490777057	0.1665510975200944	0.6873378546133346
0.3333450271729540	0.6666948625072345	0.6874000637056965
0.8334269544105219	0.6668738230556800	0.6872846963461499
0.1668170990478095	0.3333529982493560	0.8127991702731322
0.6665161710476593	0.3333443888499054	0.8125511740035878
0.1667738085099159	0.8336866200011253	0.8130729279028570
0.6666821201456012	0.8335111001676763	0.8131957566291851
0.0004805008802520	0.0004818786496796	0.8542760377610062
0.4995908856540410	0.0003562352917708	0.8544070290477866
0.0001108539459442	0.5002460416564849	0.8538201144679243
0.4998663470880770	0.5001237887812817	0.8540922479964299

0.3344157624586796	0.1683984975322698	0.9821415199436866
0.8331787777290417	0.1664480878433171	0.9796003864952514
0.3334537808214362	0.6672808151648340	0.9795782650318268
0.8332786451130790	0.6671672662016915	0.9797350256407779

(1.6) 2×2×1 supercell with the EP localized on Fe6 (-823.203 eV)

0.1804407828442546	0.0133522623623303	0.0831143203578553
0.3342048626050084	0.3200087691849950	0.0828873750180616
0.4863852277628883	0.1668918225099215	0.0829895585772178
0.6747472252833300	0.0090062751081795	0.0785492251450648
0.8331953431792603	0.3198782707365364	0.0827341615199913
0.9907753709444266	0.1647653407171966	0.0789816180791834
0.1806552005814822	0.5137339272648594	0.0828163743061207
0.3336461938213983	0.8199005941116796	0.0835758617331391
0.4861803400504136	0.6658148846917428	0.0827199197711657
0.6801167087585501	0.5133233515748712	0.0830550464416460
0.8333623721572981	0.8191207797807502	0.0826449395352771
0.9864377188476053	0.6656952491018128	0.0835710150597075
0.1529950461474759	0.1538763312726815	0.2495847588069625
0.0068015911855264	0.3566298084027149	0.2514862354857684
0.3432102318456908	0.9989824392289041	0.2503141364964631
0.6420077705902828	0.1517768186050256	0.2520627076577684
0.4986137420416094	0.3472586277667452	0.2502749151650529
0.8478425114186953	0.9955720647405645	0.2502064305302962
0.1549865023138574	0.6560763065920642	0.2500924139428209
0.0002320891976211	0.8460862230771824	0.2499834428376452
0.3481275766810896	0.5017043224338308	0.2500181772041155
0.6534276936471917	0.6527639339154313	0.2499808061761012
0.5005884122948839	0.8473011806980340	0.2498133975994773
0.8463400359713393	0.5002092415504987	0.2502034619665975
0.0136378615614119	0.1807974884573969	0.416475344017925
0.3200682296463488	0.3340716275961466	0.4171480557822184
0.1676131011647791	0.4874043209725382	0.4179052686379391
0.5125896415507935	0.1807674813421452	0.4183867720268175
0.8193588778205523	0.3334692853399375	0.4169822527695462
0.6661437913374871	0.4868714465648230	0.4172993604205121
0.0135538941760092	0.6803240742453753	0.4171963081104861
0.3197831269004441	0.8338575839557455	0.4172905323944537
0.1660248630125574	0.9868602753815644	0.4172631777011280
0.5137412572624621	0.6804643476962946	0.4169566401969628
0.8198449802882597	0.8333166765469617	0.4173044790662364
0.6666263524088242	0.9867154460395532	0.4165875673652370
0.4863861887978879	0.3198963592080345	0.5839343221735982
0.1801261887675517	0.1671469130929793	0.5835947057142231

0.3330086885075056	0.0135829028119033	0.5838061523656888
0.9865179378970771	0.3200030791159456	0.5833564731090048
0.6802381547076849	0.1667561296435776	0.5834730876871069
0.8335334165889478	0.0138133960421821	0.5832435897166263
0.4868606321029379	0.8201052830598127	0.5834818394424580
0.1804173685425616	0.6670939435153689	0.5837358857830602
0.3334814676957047	0.5138993318319770	0.5836374554022066
0.9865276548259961	0.8197684096034412	0.5836120803229303
0.6804046907226667	0.6669915177287510	0.5835383928356179
0.8332916741833529	0.5135299405282511	0.5835498881002082
0.3469745822065420	0.3470670784216588	0.7497195156005695
0.1530889985878039	0.9996400090680770	0.7498777721516025
-0.0000409578196838	0.1530141548812435	0.7496578968980171
0.8469707669480729	0.3469121888883501	0.7497579980416382
0.6531284199615097	0.0000147212551701	0.7496154480825664
0.5000008000568632	0.1529556952948026	0.7500463478623217
0.3467941278455225	0.8468886702430724	0.7498755135803130
0.1531170527016561	0.4999803302132566	0.7499265103827034
0.0001033679318755	0.6530890941763154	0.7500403680451527
0.8470710431984749	0.8468479023107757	0.7496724111512744
0.6532401186246090	0.4997721871991569	0.7498399330298624
0.5002225497479390	0.6529915366020288	0.7495559719575252
0.3200585134071433	0.4866850441393022	0.9159982410528217
0.1685023495455056	0.1803211464300220	0.9149596076329138
0.0135740708978210	0.3329112346505914	0.9162323646979307
0.8198740301067684	0.4866271221734658	0.9161648803433314
0.6673859733257288	0.1804571756337750	0.9163083286240676
0.5135862362708150	0.3330322801278661	0.9161920895580663
0.3200020205349606	0.9860167544886969	0.9165966175144801
0.1664790728770892	0.6799891672540355	0.9166054384933168
0.0137288654718931	0.8331635269104354	0.9165940692512962
0.8194451256863881	0.9856751394357576	0.9155564715904125
0.6669868143376938	0.6795034787407814	0.9159284684871635
0.5122799588470447	0.8313646863805950	0.9149054090143872
0.1674747727971692	0.3333909039729578	0.0201854279025579
0.6673337435462730	0.3329859028619471	0.0207755679441405
0.1668903425529390	0.8327485085452163	0.0218489716117256
0.6661556067724514	0.8320867206636254	0.0197275896212297
0.9991263304907991	0.0012790916269673	0.1452509238591836
0.5049912361904502	0.0028866015466988	0.1465467044940245
0.9994227718032853	0.4963590692792554	0.1470712725047292
0.4999763303046399	0.4999104554417445	0.1461310577615328
0.3328515367439655	0.1655987500942599	0.1874519079208110
0.8295453881679064	0.1624005018014029	0.1884564716489990

0.3332402372367046	0.6681403785698216	0.1870570017736732
0.8344256096287006	0.6669308710294433	0.1872246004446616
0.1663959213278817	0.3347919419052556	0.3117081797134462
0.6658317987450658	0.3333805669823395	0.3126238638114920
0.1660883209930923	0.8332831850782801	0.3128083784906299
0.6671448360023429	0.8335554052288819	0.3121561207160968
-0.0005525784300095	0.0000585505355668	0.3530343954817633
0.4996124845296180	0.0018359839293210	0.3536207502191261
0.0007262722911252	0.4996617425853005	0.3536351149423480
0.4997389219553616	0.5002098569341717	0.3537933615792886
0.3323681964624267	0.1669257292196325	0.4796071388622547
0.8333083123958518	0.1669157616923523	0.4785848423826445
0.3340082889503248	0.6677153490842994	0.4794055364998306
0.8335166856304294	0.6666546589357855	0.4792410771200332
0.1668711712056863	0.3340592464445762	0.5201403162280388
0.6662362603711184	0.3332620438684910	0.5205141942785891
0.1666822485426870	0.8335264058143285	0.5203260814497481
0.6670756082525511	0.8336432204680030	0.5201494222575461
0.0000699892331383	0.0000673307485518	0.6459784614829686
0.4999089252832142	0.0000569948198539	0.6460863521053075
0.0001179137298592	0.5001748913306878	0.6460837257631109
0.5001549630632632	0.5002867026139185	0.6460440776655706
0.3333537305503037	0.1666665451101264	0.6874294024597780
0.8333931003150384	0.1667649621460433	0.6869450623646614
0.3333474275157031	0.6667076041090803	0.6873037624730673
0.8334415963621784	0.6665334533672665	0.6872349872752666
0.1664936876126110	0.3330162281542234	0.8127858470753789
0.6668136020311952	0.3330470125677299	0.8130340514778405
0.1668025992948184	0.8331754644785524	0.8131933935050444
0.6668204109315891	0.8333545689706664	0.8124569619967754
0.0001173379679364	-0.0001610668558745	0.8540625290332787
0.5006294969445765	0.0001137035054232	0.8543505237177804
0.9999306061360429	0.4993501757404679	0.8542687076579987
0.5000177948787228	0.4996586814418665	0.8538494464986023
0.3336455412132658	0.1663298148770595	0.9795801010946448
0.8338629681001152	0.1654146900496500	0.9820655554375648
0.3332075284615933	0.6666311527199544	0.9796380640788942
0.8337104419730185	0.6664561292963627	0.9797624173330560

(1.7) 2×2×1 supercell with the EP localized on Fe7 (-823.203 eV)

0.1799403023832465	0.0141772161608395	0.0828851101325419
0.3329720495410334	0.3194192053115265	0.0830000634056613
0.4866188839717062	0.1670609605730682	0.0831296739675517
0.6807658138782259	0.0141804788422706	0.0827128093930937

0.8344024658465208	0.3208067209279700	0.0834826488425525
0.9865691692760348	0.1666871430280772	0.0830281590364600
0.1801763231009180	0.5132982329729111	0.0829179335420385
0.3350677580360610	0.8258944183026462	0.0791515167753111
0.4908301368155050	0.6655964738228608	0.0785462275972440
0.6799781272657137	0.5137312324642704	0.0835511764381652
0.8341041880558727	0.8203001401341672	0.0827542559011912
0.9861933652855034	0.6668524011770631	0.0828136254318703
0.1527616072832486	0.1514011201695237	0.2502755827589941
-0.0001897421479719	0.3462275219231970	0.2502141809376490
0.3462065737073336	-0.0006990324188832	0.2496750573053312
0.6539258602935527	0.1541904509098418	0.2499379674502258
0.5010625076266840	0.3442539347854680	0.2503066024194394
0.8473618918777563	0.0008368202307916	0.2499939720670307
0.1433887280883232	0.6502804958779997	0.2515135448335971
-0.0017294658813118	0.8463548268582849	0.2500172120356529
0.3482906495809309	0.4902329194446780	0.2521218433885127
0.6526899696026668	0.6534108032472781	0.2498339682800373
0.5043951030792213	0.8521841550731629	0.2502749884607050
0.8439456692492310	0.4988811761914420	0.2500459081126839
0.0132508521494572	0.1793607957540141	0.4172956017544705
0.3193567535944526	0.3319043187901765	0.4184220533313815
0.1666131366159279	0.4859937626096735	0.4169551171811390
0.5133510990127539	0.1792871339675655	0.4173053068879431
0.8197826723196112	0.3333332049095022	0.4172097378580633
0.6662398663923592	0.4860447676214256	0.4172984273896953
0.0126272750000229	0.6802774393945751	0.4179290961737156
0.3193103506409230	0.8329558676497293	0.4164791840651756
0.1661055566387525	0.9861091419472675	0.4171439774506511
0.5135222673528691	0.6801021206875042	0.4166322676831688
0.8197201452964551	0.8334523472298350	0.4170215964242615
0.6668427504918116	0.9867156547224507	0.4173159611236728
0.4866057787348309	0.3195030039916991	0.5838792055453732
0.1802100561648721	0.1665231109490274	0.5838952159485142
0.3329927772527496	0.0130433025948688	0.5835806931347199
0.9865945894756482	0.3198036592191105	0.5835564960191901
0.6803368515671170	0.1668504091095775	0.5836849829285850
0.8331587495202143	0.0135072525618148	0.5835599046540947
0.4863083496469556	0.8198305313795822	0.5832484184777295
0.1801337899390050	0.6665185082004486	0.5833167036885596
0.3334687477447941	0.5136306215818666	0.5834216885765445
0.9862301699163799	0.8196391243204890	0.5836542227349406
0.6799954250938844	0.6668412796817533	0.5835210940589194
0.8329820632902836	0.5133739415904603	0.5838032331632281

0.3469287109303555	0.3469845689180478	0.7500276098238339
0.1529216579041908	-0.0001513256937780	0.7497164125699416
0.0001704823343600	0.1533858110273123	0.7498231848328143
0.8468606773170443	0.3469352837518893	0.7500692744202552
0.6531014951216872	0.0001317176313091	0.7497415238236971
0.5002536292007996	0.1533180741486575	0.7499269713359221
0.3468968847566890	0.8468661591186823	0.7496855181679718
0.1530557118828350	0.5000110343167112	0.7497455647565282
0.0000033099404275	0.6530789090708981	0.7499313592249947
0.8469208376826656	0.8471489549606462	0.7495705069454821
0.6530725515023031	0.4998809420072680	0.7499263447501074
0.4998616593307978	0.6530328527894128	0.7496995431595588
0.3192843897157572	0.4867797240355922	0.9163086373993043
0.1668085603331125	0.1803825150788025	0.9161564992090691
0.0132398962200180	0.3331882006500743	0.9162162354295745
0.8198600515101785	0.4863978446024574	0.9165783515526561
0.6666908229553599	0.1804470759155525	0.9166111331437146
0.5137740054084050	0.3338090310721586	0.9165761253986382
0.3194769692246432	0.9879618816741074	0.9150621086560001
0.1669645031271291	0.6804938712031366	0.9163393632337861
0.0131398143310022	0.8332553608783009	0.9159735220213120
0.8203433297575062	0.9873484213285441	0.9159662861284668
0.6684370412372920	0.6807571501134736	0.9149525533147187
0.5141580030541931	0.8336664378090858	0.9156541671064541
0.1668715934222857	0.3343206105175665	0.0208119256236669
0.6672043287649173	0.3341028434747369	0.0218976386689325
0.1665627145635546	0.8340134638931460	0.0202741500122934
0.6678138218966686	0.8339765605942283	0.0198263084356461
0.0000312894991189	0.0000487088667445	0.1461497506626485
0.4986076285094831	-0.0021914977185070	0.1453549760727263
0.0036727798233245	0.5031465089508335	0.1471329155128422
0.4969283471601493	0.5019995392500566	0.1465666310716976
0.3344150762237307	0.1673053696337763	0.1874168892375196
0.8330933986775881	0.1675963515671829	0.1871466403087672
0.3376520229252710	0.6671502112757510	0.1885588263890579
0.8317371538635885	0.6650934455602068	0.1870576570315186
0.1666359688159629	0.3325252533120870	0.3126114475112980
0.6667422954134856	0.3328545807635965	0.3127930605783986
0.1652838703942709	0.8317265486416150	0.3117059863718958
0.6666481562890331	0.8338269486133064	0.3121875822795406
0.0000075067464108	-0.0003551224596866	0.3538346906861075
0.5001093500371164	-0.0005420685486879	0.3531022735570275
0.0003701118843994	0.5011660673225227	0.3536376836518344
0.4982832136111495	0.4978906176778510	0.3536572370627004

0.3332639973678993	0.1655453733811191	0.4796116566847139
0.8335728265113410	0.1670648616954540	0.4792839499108558
0.3332416605186200	0.6664938015523643	0.4785261089250594
0.8323641917660833	0.6663645898681753	0.4794708781243160
0.1669195866951354	0.3331066444247300	0.5204963220178235
0.6666056142736816	0.3332454901086306	0.5203204833814141
0.1660880074269769	0.8328854304083420	0.5201346624958915
0.6664839085128968	0.8335559837732971	0.5201712205211101
-0.0001879240812603	-0.0001100439464554	0.6460322068455957
0.5000352494393369	0.0000138412734538	0.6460426870721599
-0.0000736693854934	0.4999760703598382	0.6460965068698928
0.5000372389218162	0.4999006222966720	0.6461473402886220
0.3333331015881238	0.1666752275893721	0.6874029664282384
0.8334045815611612	0.1668341278499643	0.6872630228391917
0.3332460683119803	0.6666243396504840	0.6869196040150074
0.8332924074015842	0.6666202106206539	0.6873501122148944
0.1668210642133878	0.3336604616530501	0.8130632967338742
0.6667178812480618	0.3334951493407611	0.8131991249237243
0.1668685380221367	0.8333810105347382	0.8128507276997466
0.6665590395547113	0.8333388684809691	0.8125570506653629
0.0001683137027034	0.0002285136297696	0.8538026013882104
0.5000005140640470	0.0001417230555826	0.8541162122245093
0.0005272890201632	0.5004778505893517	0.8542827047796479
0.4996653366332498	0.5003305147312374	0.8543913775575532
0.3335205269644904	0.1672215299574986	0.9795518001093745
0.8333999204704463	0.1671316252419470	0.9797218243848020
0.3344584907096519	0.6683468630124771	0.9821348151368329
0.8333030805986977	0.6665219397950024	0.9796130738634037

(1.8) 2×2×1 supercell with the EP localized on Fe8 (-823.203 eV)

0.1804688210289438	0.0135428121035045	0.0830392863644579
0.3329064699828747	0.3195175050980105	0.0831679212680871
0.4857211288452994	0.1657051293482581	0.0828733256244318
0.6796210162550848	0.0137765212946428	0.0827588519216891
0.8330542285894211	0.3192903201286571	0.0827935420517156
0.9862056228194790	0.1662482962312637	0.0836118757216322
0.1792329718097773	0.5134981425077173	0.0835745777098622
0.3332085128536234	0.8198535404892963	0.0830938128629977
0.4856945753510042	0.6665581300187542	0.0826674417360239
0.6740081641521453	0.5090829130859811	0.0790746525210373
0.8342013714895727	0.8251666935306393	0.0785102136478971
0.9865952057657720	0.6667189322025792	0.0827395733024040
0.1558548146834787	0.1568356510791357	0.2503819810174968
0.0011771328513586	0.3450693757649331	0.2500673891825433

0.3486853756560084	0.0014337837057139	0.2503193750257469
0.6536204078191568	0.1519337547170364	0.2500125781228573
0.5008530869455493	0.3470521645178534	0.2496107799894222
0.8467092201676100	0.9994329003885964	0.2498434719232688
0.1538010372228035	0.6536775740368885	0.2502083380478186
0.0096981132669135	0.8580144084460949	0.2521497152293072
0.3459696241980731	0.4998704302800757	0.2500001668783702
0.6479026038712951	0.6523342749862560	0.2502270819789802
0.4992786578501296	0.8465948075009730	0.2500334812558645
0.8498565265240005	0.4931650256428848	0.2514695477669338
0.0141324867256392	0.1803318871724747	0.4173309302890307
0.3208935543044821	0.3341222777156855	0.4172997643631854
0.1668849851880815	0.4866114253829500	0.4171909789662324
0.5140344318587373	0.1800922729218769	0.4171205236102397
0.8198388134517733	0.3324690197414959	0.4179072022677376
0.6672901863783832	0.4865316129523935	0.4164422676038130
0.0141791346154702	0.6807629900464061	0.4170184121490151
0.3207743000119911	0.8339781726840423	0.4173409195099846
0.1682199647084012	0.9875164631123040	0.4184374156349223
0.5135164134764072	0.6802662455383371	0.4173069392463628
0.8200933036907163	0.8335014751494891	0.4166440403748698
0.6667402165772877	0.9863663176919870	0.4170092649809789
0.4870554136596930	0.3199864831192112	0.5835781697551675
0.1805942250918120	0.1670812115121215	0.5838410226427909
0.3335488251291804	0.0137132265498380	0.5839529742365949
0.9866675924594531	0.3196507536615946	0.5837529592555731
0.6804141952721138	0.1666171502469981	0.5836523736495681
0.8333026162161811	0.0132219914451482	0.5835136174886684
0.4866137653302964	0.8196833171870453	0.5835754287702104
0.1802555033647508	0.6667821936836223	0.5835834304292673
0.3332996747781404	0.5135961529022705	0.5836125246435470
0.9865559585932836	0.8198465040100457	0.5835124446960539
0.6802984340129445	0.6665830787049358	0.5832755115983813
0.8335173517540242	0.5136017224745705	0.5833528065116381
0.3465306285826952	0.3468581158570710	0.7498852423175943
0.1529726450489797	-0.0000488516690007	0.7500795400673105
0.0000856506330506	0.1531583483269273	0.7499037191873981
0.8468485790677722	0.3468218116927292	0.7499268985436197
0.6527641068640824	0.9997308824804193	0.7495703872380396
0.5000280946000739	0.1529520817584877	0.7497447762584538
0.3465226929674933	0.8467149235526712	0.7498594333469353
0.1529758316190497	0.4998319017373967	0.7500516326121202
-0.0001296598168540	0.6529239461977977	0.7497913621937120
0.8468722306465736	0.8468147320561780	0.7496594643650635

0.6530002832881249	0.4999423145683451	0.7496358963068505
0.4997175872997600	0.6528426827021949	0.7496996465449582
0.3193913517546503	0.4860887271454116	0.9166461369394704
0.1659698133031422	0.1798789770581722	0.9166525331182731
0.0134890958000972	0.3334053292135836	0.9166231635288079
0.8192695811180881	0.4863418254871648	0.9162198327410226
0.6665953419147410	0.1798385195516478	0.9159786688505347
0.5118162320169101	0.3314112978339126	0.9150187852908350
0.3194042434843170	0.9862594750061152	0.9162368359249410
0.1666762324193947	0.6799497964136522	0.9162036088418904
0.0130980498931549	0.8325210061275211	0.9162768097737628
0.8190291571776372	0.9876009371156315	0.9149103658057698
0.6661104003628902	0.6803641068227833	0.9155826370470976
0.5124773552839892	0.8328782999788235	0.9159654334553238
0.1658379606749021	0.3329867629187023	0.0218942694857124
0.6658653841475102	0.3324675723664777	0.0201804845430630
0.1656319770956418	0.8325831440420707	0.0208186978465377
0.6658358434587768	0.8337773887819006	0.0197418830010742
0.9978255325411370	0.9948671554762055	0.1465721389698137
0.4999376066118918	0.0000333695679439	0.1461600035183656
0.9969271343252100	0.5004815629716193	0.1470615540536633
0.5021943323295853	0.5008698062775312	0.1452917172800254
0.3327332107550420	0.1671568402487001	0.1874820733188965
0.8349139226347322	0.1667457167640627	0.1870697666007205
0.3324893501110510	0.6656005637302139	0.1872586265264312
0.8329067578619196	0.6703761322080756	0.1884553540613692
0.1672812731416923	0.3339852672239739	0.3128243177118959
0.6683928192687707	0.3336502507244524	0.3117025426986266
0.1675502335497231	0.8342315952522285	0.3126591324025139
0.6663751499718568	0.8329199368440757	0.3122047941550894
0.0022388726488372	0.0004808190941127	0.3536796345965154
0.5004898881228304	0.0003778936429616	0.3538133694753137
0.9990113134176180	0.4993838974557756	0.3536527209537861
0.5007132402621728	0.5007057020307814	0.3530365080072902
0.3345923750155301	0.1677609120888284	0.4796188531615834
0.8337447709329205	0.1661182652439527	0.4794451512882382
0.3332134917733420	0.6666301006874562	0.4792778217468046
0.8336692182138871	0.6668584579624424	0.4786122507546806
0.1668718024812005	0.3334279867854192	0.5203508927393228
0.6672258424135079	0.3332611934751053	0.5201283326331304
0.1670640181158571	0.8338662076117315	0.5205455008341240
0.6665885155978422	0.8330411909561160	0.5201937019250958
0.0001796911878053	0.0001387283451024	0.6461336654102745
0.5001587420757003	0.9999177678354106	0.6460649892618543

0.0000678709437484	0.4999490995617708	0.6460891643929663
0.5000223022642057	0.5000012923189769	0.6459677131406507
0.3332814219750445	0.1666133771284754	0.6874365300961125
0.8333568585470990	0.1666290252633196	0.6873311467471304
0.3330605610876027	0.6665272553794210	0.6872695153147012
0.8333409754613964	0.6665766274059204	0.6869707783223560
0.1663764655436639	0.3331454634449986	0.8132328149606485
0.6665080589483003	0.3334061448136708	0.8127768218847098
0.1661895928097746	0.8330724575089173	0.8130602633273963
0.6664905753104324	0.8330783323399571	0.8124691185574383
0.9994619013479793	0.9992979009182145	0.8543784194700225
0.4995910741060686	0.9998422240628565	0.8538834903211870
0.9993721240614637	0.4999387439532892	0.8542842659439510
0.4996706868084139	0.4997163369535984	0.8540624803207639
0.3326499609662962	0.1662314425048197	0.9796235472810000
0.8333647248481675	0.1667078296625477	0.9796436692058946
0.3326696980058504	0.6661220926228000	0.9797990766856863
0.8315037952475884	0.6660731208148113	0.9820383429411141

(1.9) $2\times 2\times 1$ supercell with the EP transfer from initial to final state with $d_{\text{Fe-Fe}} = 2.91 \text{ \AA}$ as an example

Initial coordinate: 0 (-823.203 eV)

0.1775296638988950	0.0098864594904548	0.0828756767353683
0.3237655789899154	0.3086449919922368	0.0810497242043729
0.4867062314112072	0.1672482587193708	0.0834417002043438
0.6797044910517636	0.0146507356987682	0.0833828900821327
0.8341416689254200	0.3200373828950028	0.0833142708917892
0.9846867444401258	0.1652156433799164	0.0829975223989163
0.1795423752553227	0.5129228529914100	0.0831521626640514
0.3320915512990337	0.8215750834534763	0.0833208442786446
0.4834659313677361	0.6735489851535839	0.0819554139040291
0.6853848919500241	0.5141544765727362	0.0831011367232782
0.8325490271359929	0.8196104327404483	0.0837648817504069
0.9873586119486656	0.6667772493935004	0.0833941155018580
0.1528792971052447	0.1532647710212051	0.2502385520357527
0.0001361795970754	0.3469022916067299	0.2502199740925874
0.3471338494210391	0.0005587663780779	0.2497244969112869
0.6537020262266630	0.1529650165925935	0.2505471755176473
0.4991485772838358	0.3415963690244834	0.2548001824126955
0.8476218552150809	0.0010533605042919	0.2505017298924438
0.1541145589922263	0.6532367611675850	0.2498293369883546
0.0004659752327347	0.8472443708833877	0.2501553048215922
0.3467433995666365	0.5000738319695621	0.2505474682227289
0.6592869786614727	0.6577158945093013	0.2542094907475846
0.5002228521719964	0.8474922673814852	0.2506089449092809

0.8476447881799641	0.5001921596368938	0.2506614457647094
0.0139205600202965	0.1805537760587902	0.4170988183346432
0.3202558961142006	0.3343232803751154	0.4170228118099049
0.1666842970689719	0.4868828698125789	0.4171130697216024
0.5142729399263259	0.1791930494011667	0.4184359997614897
0.8208486385723802	0.3338833547886313	0.4173624923659987
0.6672361444277169	0.4864531115360849	0.4177113416213291
0.0139005388164459	0.6806893680596120	0.4166865421384994
0.3198209623926332	0.8334069829456145	0.4167552540120243
0.1672971522429923	0.9869459534100010	0.4166789610094079
0.5140272588903079	0.6804387216940385	0.4170819112932807
0.8214974693792164	0.8354196535063761	0.4183348324345986
0.6666789652926567	0.9869616537647450	0.4173988793156193
0.4864310097457898	0.3198891938207646	0.5836376979246298
0.1803202981534713	0.1667735899863389	0.5832481665860684
0.3332134000390389	0.0135332658421483	0.5834132026133083
0.9867718255044793	0.3199340831387514	0.5834537266333528
0.6805250670662757	0.1669609542558444	0.5837754569707568
0.8332267642033445	0.0137074080913919	0.5836236653463857
0.4864270776793146	0.8197909909408917	0.5834418813276129
0.1803025733414644	0.6668407349785960	0.5832618950710048
0.3334093800484682	0.5137296429258104	0.5835630520175921
0.9867337392995433	0.8198119721166992	0.5834483519124116
0.6802673525505322	0.6667705475794102	0.5837095452847549
0.8335580150881333	0.5138255744615566	0.5836177222330934
0.3467987720616228	0.3467060861725801	0.7498225915668363
0.1527474486570918	-0.0005431710728039	0.7494708033881753
-0.0002560753084692	0.1528139315218612	0.7493983429406718
0.8467706731534216	0.3469128887600286	0.7497277543877467
0.6528942567479223	-0.0000974879837472	0.7497082578780206
0.5000594209397866	0.1533265034044905	0.7497605181405430
0.3466551202293647	0.8469067308033401	0.7495717193305694
0.1530683119156481	0.4997688924859817	0.7497495016539822
0.0000560544531341	0.6529826717742016	0.7497121288580944
0.8462763173851079	0.8465800080564854	0.7498078043120295
0.6530772955800839	0.5000119901309723	0.7500601033695350
0.4997845323492358	0.6529354100369910	0.7500398624858584
0.3192117162197118	0.4859021570113096	0.9163650252358452
0.1651721055526004	0.1790650694685648	0.9148164943896260
0.0125867552246470	0.3325246306424404	0.9159744464420804
0.8198782709104875	0.4862877048420708	0.9160188556483588
0.6667076596266865	0.1801814417126341	0.9162857452775538
0.5132926104252787	0.3330014424202091	0.9166008889016891
0.3191919445257074	0.9862069689406185	0.9159683919218028

0.1664602115938064	0.6799566929977154	0.9161692079887770
0.0124056449156965	0.8323422885269557	0.9160262775081687
0.8193150413586877	0.9863633455343671	0.9162751094278396
0.6660209802785088	0.6799535528698977	0.9169612669398175
0.5135116690824880	0.8341256034681285	0.9154734765860518
0.1658613387780607	0.3324253209601774	0.0206408150735755
0.6671008119136995	0.3336931574921195	0.0210839890381484
0.1660011491376315	0.8326176500164478	0.0205097397101421
0.6650121435347204	0.8329662476581986	0.0217139638821349
0.0007255344138573	-0.0003982207279100	0.1458685292212673
0.4984103658551758	0.0000012884012070	0.1462637113840655
0.0008965475889059	0.5010443652462268	0.1461210185183964
0.5004678184311419	0.4963628397954032	0.1448408184772301
0.3355250975229344	0.1719380382540623	0.1866857791769887
0.8334016379932808	0.1666736371503254	0.1871765450643681
0.3364129753582219	0.6663314985143760	0.1863168929820630
0.8311514842868845	0.6659029296524336	0.1880434909416791
0.1677468494337253	0.3342376406521909	0.3124984467130730
0.6675116787348937	0.3329740891353585	0.3135659577516050
0.1675166167168471	0.8338068924952748	0.3114477422137347
0.6674292569975158	0.8343113565719164	0.3131796530508686
0.0006518230294153	0.0005922125459739	0.3537081125819618
0.4999530551587240	0.0000930291573783	0.3537086167300447
0.0006275410552356	0.5006528064440082	0.3535606797177064
0.5018529525503587	0.5007339325229684	0.3512350424245297
0.3337931276624126	0.1675142623408463	0.4789247879906160
0.8337104418571557	0.1669269940088066	0.4794718391529229
0.3339570214894712	0.6668478707743578	0.4790513362604233
0.8336153708549686	0.6670775601737631	0.4792613949473643
0.1671159726086883	0.3336894504866775	0.5202500778434559
0.6667875980951681	0.3336323032634859	0.5208337791220042
0.1668947176160828	0.8335670420349146	0.5200942366772657
0.6667714498586370	0.8333032266435788	0.5205800475749099
0.0000097631618688	0.0000422257116815	0.6459223868329012
0.4999390031365915	0.0000263768424713	0.6459973324358805
0.0002308008321663	0.5001029500990144	0.6460280147125723
0.4999693463304537	0.5000645874411851	0.6463751552508293
0.3331355202075558	0.1664159313585710	0.6871669689467332
0.8331065435251372	0.1666074343043052	0.6872732068786471
0.3332458045117614	0.6666181302590317	0.6872572126401315
0.8333110929339359	0.6666025555827786	0.6873615556322887
0.1662774574911925	0.3326399350664311	0.8127695584683217
0.6667842309186296	0.3335152724278619	0.8130914676261249
0.1664865289154772	0.8331218193225558	0.8129802157728003

0.6660807384389682	0.8332598137252860	0.8132739493633726
-0.0012399719726091	-0.0012762328088864	0.8537335480056757
0.4996265554645943	0.0004122072708792	0.8538943488150317
0.0001889714992081	0.4999111558555656	0.8540467979969809
0.4996436641813404	0.4996675323490507	0.8547484041180669
0.3311683005899825	0.1660942928734377	0.9795771768475786
0.8328920031905034	0.1661190061694215	0.9795323169220234
0.3343067467317206	0.6672475136796856	0.9797520078929414
0.8325931793074005	0.6657843976323746	0.9802951296436833

Interpolating coordinate: 0.167 (-823.188 eV)

0.176927357	0.009762812	0.082210468
0.325465420	0.311397072	0.080597592
0.486658780	0.167158225	0.083287001
0.679601487	0.014472060	0.083365042
0.833965386	0.320019494	0.083222278
0.984825686	0.165430354	0.082896506
0.179528582	0.513067074	0.083056169
0.332236475	0.821204307	0.083193223
0.483892595	0.672330463	0.082197285
0.684527666	0.514042025	0.083049434
0.832567002	0.819598412	0.083617794
0.987049833	0.666608149	0.083268457
0.152049914	0.153161517	0.250195368
-0.000008711	0.346889893	0.250136009
0.347594444	-0.000638782	0.249966730
0.653735988	0.153137488	0.250439311
0.500903505	0.344374927	0.254328659
0.847348612	0.000886905	0.250367111
0.154030934	0.653064891	0.249822595
0.000522544	0.847245584	0.250019201
0.346756566	0.500020092	0.250404866
0.658712536	0.657606415	0.253537156
0.500393043	0.847132924	0.250480189
0.847806824	0.500438564	0.250556947
0.013864750	0.180557822	0.417094156
0.320240601	0.334241284	0.416926975
0.166696470	0.486853276	0.417058243
0.514268973	0.179494371	0.418148974
0.820851933	0.333948689	0.417315507
0.667423982	0.486680474	0.417792515
0.013947146	0.680652669	0.416718384
0.319837648	0.833298813	0.416916572
0.167312990	0.986929044	0.416585768

0.514063289	0.680466848	0.417091017
0.821430904	0.835269562	0.418129583
0.666723755	0.986953357	0.417323563
0.486451469	0.319897112	0.583572464
0.180308405	0.166755829	0.583209721
0.333271817	0.013575266	0.583353227
0.986749433	0.319927528	0.583440089
0.680473975	0.166966467	0.583704606
0.833237506	0.013722003	0.583585460
0.486489699	0.819797788	0.583460129
0.180331061	0.666834797	0.583302289
0.333379386	0.513668920	0.583521185
0.986802746	0.819865723	0.583431770
0.680323564	0.666846108	0.583692786
0.833569084	0.513842314	0.583637937
0.346770360	0.346721990	0.749753439
0.152769367	-0.000472704	0.749459577
-0.000276703	0.152821362	0.749406645
0.846699653	0.346878427	0.749711322
0.652873593	-0.000115026	0.749719127
0.499992249	0.153250115	0.749720470
0.346651366	0.846893996	0.749596811
0.152991686	0.499775457	0.749694747
0.000015882	0.652977744	0.749688458
0.846288094	0.846627674	0.749777864
0.653019740	0.499990242	0.750013974
0.499804485	0.652965260	0.749976154
0.319142752	0.486176422	0.916090494
0.165294278	0.179273573	0.914902683
0.012518471	0.332567364	0.915929750
0.819748570	0.486277894	0.916012010
0.666667470	0.180133707	0.916218991
0.513212378	0.332898488	0.916514188
0.319160760	0.986217626	0.915981263
0.166426273	0.679919540	0.916111215
0.012257750	0.832180336	0.915822692
0.819274821	0.986311489	0.916277967
0.665971284	0.679921155	0.916859927
0.513454138	0.833982614	0.915617651
0.165825233	0.332648048	0.020458428
0.666817300	0.333502599	0.020991823
0.165946748	0.832590407	0.020426361
0.665096189	0.832962938	0.021701079
0.000945429	-0.000184625	0.145726150

0.498156712	0.000103133	0.146357508
0.000715119	0.500888748	0.146086499
0.499997555	0.496111169	0.145096341
0.335080196	0.171707450	0.186942536
0.833242832	0.166524295	0.187135134
0.336164917	0.666431750	0.186413000
0.831386939	0.666136497	0.187904544
0.167518613	0.334068973	0.312409939
0.667515358	0.333218248	0.313369160
0.167670986	0.833826377	0.311443512
0.667420927	0.834305461	0.313088148
0.000689133	0.000673149	0.353555614
0.499806403	0.000007241	0.353657790
0.000611070	0.500661633	0.353563886
0.501936003	0.500743392	0.351607627
0.333790851	0.167455372	0.478826343
0.833639771	0.166926351	0.479399881
0.333938842	0.666768931	0.479084332
0.833799331	0.667238468	0.479282126
0.167039086	0.333619163	0.520199169
0.666841525	0.333714089	0.520742709
0.166974576	0.833556093	0.520059970
0.666805503	0.833366627	0.520500727
-0.000003115	0.000046165	0.645888567
0.499957659	0.000032747	0.645968643
0.000223374	0.500102129	0.646006424
0.499996871	0.500093164	0.646294134
0.333137336	0.166446005	0.687091344
0.833086293	0.166602014	0.687235510
0.333239715	0.666631812	0.687237315
0.833277011	0.666610460	0.687333434
0.166283361	0.332718135	0.812688505
0.666635406	0.333422138	0.813035394
0.166445082	0.833159511	0.812920870
0.666087348	0.833228448	0.813220335
-0.001128721	-0.001112333	0.853741820
0.499528672	0.000310784	0.853918309
0.000039844	0.499881554	0.853987006
0.499569404	0.499579299	0.854646929
0.331178905	0.166073907	0.979955764
0.832811159	0.166110319	0.979524630
0.334099073	0.667137165	0.979698933
0.832549978	0.665852691	0.980135964

Interpolating coordinate: 0.333 (-823.145 eV)

0.176325049	0.009639164	0.081545260
0.327165261	0.314149151	0.080145460
0.486611329	0.167068192	0.083132301
0.679498484	0.014293384	0.083347194
0.833789104	0.320001604	0.083130285
0.984964627	0.165645064	0.082795491
0.179514788	0.513211295	0.082960176
0.332381400	0.820833531	0.083065603
0.484319258	0.671111942	0.082439155
0.683670440	0.513929574	0.082997732
0.832584977	0.819586392	0.083470705
0.986741054	0.666439048	0.083142799
0.151220531	0.153058263	0.250152185
-0.000153602	0.346877494	0.250052045
0.348055038	-0.001836330	0.250208963
0.653769949	0.153309960	0.250331446
0.502658433	0.347153485	0.253857135
0.847075368	0.000720449	0.250232493
0.153947309	0.652893021	0.249815852
0.000579114	0.847246797	0.249883098
0.346769733	0.499966351	0.250262264
0.658138094	0.657496936	0.252864821
0.500563233	0.846773582	0.250351434
0.847968861	0.500684969	0.250452448
0.013808940	0.180561869	0.417089493
0.320225307	0.334159287	0.416831139
0.166708643	0.486823683	0.417003416
0.514265005	0.179795692	0.417861948
0.820855227	0.334014023	0.417268521
0.667611819	0.486907837	0.417873688
0.013993753	0.680615970	0.416750226
0.319854333	0.833190643	0.417077890
0.167328828	0.986912135	0.416492575
0.514099319	0.680494975	0.417100122
0.821364338	0.835119471	0.417924334
0.666768544	0.986945060	0.417248247
0.486471928	0.319905030	0.583507231
0.180296512	0.166738069	0.583171275
0.333330233	0.013617267	0.583293251
0.986727040	0.319920972	0.583426451
0.680422883	0.166971981	0.583633755
0.833248247	0.013736597	0.583547255
0.486552320	0.819804586	0.583478377

0.180359550	0.666828859	0.583342682
0.333349391	0.513608198	0.583479318
0.986871752	0.819919474	0.583415188
0.680379776	0.666921669	0.583676027
0.833580152	0.513859053	0.583658151
0.346741947	0.346737895	0.749684287
0.152791286	-0.000402237	0.749448350
-0.000297331	0.152828792	0.749414946
0.846628633	0.346843966	0.749694889
0.652852929	-0.000132563	0.749729996
0.499925077	0.153173727	0.749680422
0.346647612	0.846881261	0.749621902
0.152915060	0.499782021	0.749639992
-0.000024291	0.652972817	0.749664787
0.846299870	0.846675340	0.749747923
0.652962185	0.499968494	0.749967844
0.499824438	0.652995111	0.749912446
0.319073787	0.486450687	0.915815962
0.165416450	0.179482077	0.914988871
0.012450186	0.332610097	0.915885053
0.819618869	0.486268084	0.916005164
0.666627280	0.180085972	0.916152236
0.513132146	0.332795534	0.916427488
0.319129575	0.986228284	0.915994133
0.166392333	0.679882387	0.916053222
0.012109855	0.832018383	0.915619106
0.819234600	0.986259632	0.916280825
0.665921588	0.679888756	0.916758588
0.513396607	0.833839625	0.915761825
0.165789128	0.332870775	0.020276041
0.666533787	0.333312041	0.020899658
0.165892347	0.832563164	0.020342982
0.665180235	0.832959628	0.021688194
0.001165323	0.000028971	0.145583771
0.497903059	0.000204977	0.146451305
0.000533691	0.500733130	0.146051979
0.499527292	0.495859498	0.145351864
0.334635295	0.171476862	0.187199293
0.833084027	0.166374953	0.187093724
0.335916858	0.666532001	0.186509106
0.831622393	0.666370063	0.187765598
0.167290376	0.333900304	0.312321431
0.667519037	0.333462408	0.313172362
0.167825356	0.833845862	0.311439283

0.667412596	0.834299565	0.312996644
0.000726444	0.000754085	0.353403115
0.499659751	-0.000078547	0.353606963
0.000594600	0.500670459	0.353567092
0.502019053	0.500752851	0.351980212
0.333788574	0.167396481	0.478727898
0.833569101	0.166925708	0.479327922
0.333920662	0.666689990	0.479117327
0.833983291	0.667399376	0.479302857
0.166962199	0.333548875	0.520148259
0.666895452	0.333795875	0.520651638
0.167054434	0.833545144	0.520025703
0.666839556	0.833430028	0.520421406
-0.000015994	0.000050105	0.645854746
0.499976315	0.000039117	0.645939953
0.000215948	0.500101308	0.645984833
0.500024395	0.500121741	0.646213112
0.333139152	0.166476079	0.687015720
0.833066042	0.166596593	0.687197813
0.333233626	0.666645494	0.687217417
0.833242929	0.666618364	0.687305313
0.166289264	0.332796335	0.812607452
0.666486581	0.333329003	0.812979320
0.166403635	0.833197203	0.812861524
0.666093958	0.833197083	0.813166721
-0.001017470	-0.000948432	0.853750093
0.499430788	0.000209361	0.853942270
-0.000109284	0.499851952	0.853927215
0.499495144	0.499491067	0.854545455
0.331189510	0.166053522	0.980334351
0.832730314	0.166101632	0.979516944
0.333891399	0.667026816	0.979645858
0.832506777	0.665920984	0.979976798

Interpolating coordinate: 0.417 (-823.113 eV)

0.176325049	0.009639164	0.081545260
0.327165261	0.314149151	0.080145460
0.486611329	0.167068192	0.083132301
0.679498484	0.014293384	0.083347194
0.833789104	0.320001604	0.083130285
0.984964627	0.165645064	0.082795491
0.179514788	0.513211295	0.082960176
0.332381400	0.820833531	0.083065603
0.484319258	0.671111942	0.082439155

0.683670440	0.513929574	0.082997732
0.832584977	0.819586392	0.083470705
0.986741054	0.666439048	0.083142799
0.151220531	0.153058263	0.250152185
-0.000153602	0.346877494	0.250052045
0.348055038	-0.001836330	0.250208963
0.653769949	0.153309960	0.250331446
0.502658433	0.347153485	0.253857135
0.847075368	0.000720449	0.250232493
0.153947309	0.652893021	0.249815852
0.000579114	0.847246797	0.249883098
0.346769733	0.499966351	0.250262264
0.658138094	0.657496936	0.252864821
0.500563233	0.846773582	0.250351434
0.847968861	0.500684969	0.250452448
0.013808940	0.180561869	0.417089493
0.320225307	0.334159287	0.416831139
0.166708643	0.486823683	0.417003416
0.514265005	0.179795692	0.417861948
0.820855227	0.334014023	0.417268521
0.667611819	0.486907837	0.417873688
0.013993753	0.680615970	0.416750226
0.319854333	0.833190643	0.417077890
0.167328828	0.986912135	0.416492575
0.514099319	0.680494975	0.417100122
0.821364338	0.835119471	0.417924334
0.666768544	0.986945060	0.417248247
0.486471928	0.319905030	0.583507231
0.180296512	0.166738069	0.583171275
0.333330233	0.013617267	0.583293251
0.986727040	0.319920972	0.583426451
0.680422883	0.166971981	0.583633755
0.833248247	0.013736597	0.583547255
0.486552320	0.819804586	0.583478377
0.180359550	0.666828859	0.583342682
0.333349391	0.513608198	0.583479318
0.986871752	0.819919474	0.583415188
0.680379776	0.666921669	0.583676027
0.833580152	0.513859053	0.583658151
0.346741947	0.346737895	0.749684287
0.152791286	-0.000402237	0.749448350
-0.000297331	0.152828792	0.749414946
0.846628633	0.346843966	0.749694889
0.652852929	-0.000132563	0.749729996

0.499925077	0.153173727	0.749680422
0.346647612	0.846881261	0.749621902
0.152915060	0.499782021	0.749639992
-0.000024291	0.652972817	0.749664787
0.846299870	0.846675340	0.749747923
0.652962185	0.499968494	0.749967844
0.499824438	0.652995111	0.749912446
0.319073787	0.486450687	0.915815962
0.165416450	0.179482077	0.914988871
0.012450186	0.332610097	0.915885053
0.819618869	0.486268084	0.916005164
0.666627280	0.180085972	0.916152236
0.513132146	0.332795534	0.916427488
0.319129575	0.986228284	0.915994133
0.166392333	0.679882387	0.916053222
0.012109855	0.832018383	0.915619106
0.819234600	0.986259632	0.916280825
0.665921588	0.679888756	0.916758588
0.513396607	0.833839625	0.915761825
0.165789128	0.332870775	0.020276041
0.666533787	0.333312041	0.020899658
0.165892347	0.832563164	0.020342982
0.665180235	0.832959628	0.021688194
0.001165323	0.000028971	0.145583771
0.497903059	0.000204977	0.146451305
0.000533691	0.500733130	0.146051979
0.499527292	0.495859498	0.145351864
0.334635295	0.171476862	0.187199293
0.833084027	0.166374953	0.187093724
0.335916858	0.666532001	0.186509106
0.831622393	0.666370063	0.187765598
0.167290376	0.333900304	0.312321431
0.667519037	0.333462408	0.313172362
0.167825356	0.833845862	0.311439283
0.667412596	0.834299565	0.312996644
0.000726444	0.000754085	0.353403115
0.499659751	-0.000078547	0.353606963
0.000594600	0.500670459	0.353567092
0.502019053	0.500752851	0.351980212
0.333788574	0.167396481	0.478727898
0.833569101	0.166925708	0.479327922
0.333920662	0.666689990	0.479117327
0.833983291	0.667399376	0.479302857
0.166962199	0.333548875	0.520148259

0.666895452	0.333795875	0.520651638
0.167054434	0.833545144	0.520025703
0.666839556	0.833430028	0.520421406
-0.000015994	0.000050105	0.645854746
0.499976315	0.000039117	0.645939953
0.000215948	0.500101308	0.645984833
0.500024395	0.500121741	0.646213112
0.333139152	0.166476079	0.687015720
0.833066042	0.166596593	0.687197813
0.333233626	0.666645494	0.687217417
0.833242929	0.666618364	0.687305313
0.166289264	0.332796335	0.812607452
0.666486581	0.333329003	0.812979320
0.166403635	0.833197203	0.812861524
0.666093958	0.833197083	0.813166721
-0.001017470	-0.000948432	0.853750093
0.499430788	0.000209361	0.853942270
-0.000109284	0.499851952	0.853927215
0.499495144	0.499491067	0.854545455
0.331189510	0.166053522	0.980334351
0.832730314	0.166101632	0.979516944
0.333891399	0.667026816	0.979645858
0.832506777	0.665920984	0.979976798

Interpolating coordinate: 0.433 (-823.106 eV)

0.175963665	0.009564975	0.081146135
0.328185166	0.315800399	0.079874180
0.486582858	0.167014172	0.083039481
0.679436682	0.014186178	0.083336485
0.833683334	0.319990871	0.083075089
0.985047992	0.165773890	0.082734881
0.179506512	0.513297827	0.082902580
0.332468354	0.820611065	0.082989030
0.484575256	0.670380829	0.082584278
0.683156105	0.513862103	0.082966710
0.832595762	0.819579180	0.083382452
0.986555787	0.666337587	0.083067404
0.150722901	0.152996311	0.250126275
-0.000240536	0.346870055	0.250001666
0.348331394	-0.002554859	0.250354303
0.653790326	0.153413443	0.250266727
0.503711390	0.348820620	0.253574221
0.846911422	0.000620575	0.250151722
0.153897135	0.652789899	0.249811807

0.000613055	0.847247525	0.249801436
0.346777633	0.499934107	0.250176703
0.657793428	0.657431249	0.252461420
0.500665348	0.846557976	0.250274180
0.848066083	0.500832812	0.250389749
0.013775454	0.180564297	0.417086696
0.320216130	0.334110089	0.416773637
0.166715947	0.486805927	0.416970519
0.514262625	0.179976485	0.417689732
0.820857204	0.334053224	0.417240330
0.667724521	0.487044254	0.417922391
0.014021717	0.680593951	0.416769331
0.319864344	0.833125740	0.417174680
0.167338331	0.986901990	0.416436659
0.514120937	0.680511851	0.417105586
0.821324399	0.835029416	0.417801185
0.666795417	0.986940081	0.417203057
0.486484203	0.319909781	0.583468091
0.180289376	0.166727412	0.583148208
0.333365283	0.013642467	0.583257265
0.986713605	0.319917039	0.583418268
0.680392228	0.166975289	0.583591244
0.833254692	0.013745354	0.583524331
0.486589893	0.819808664	0.583489326
0.180376643	0.666825296	0.583366918
0.333331395	0.513571764	0.583454198
0.986913156	0.819951724	0.583405238
0.680413503	0.666967006	0.583665972
0.833586793	0.513869097	0.583670279
0.346724900	0.346747437	0.749642795
0.152804437	-0.000359957	0.749441614
-0.000309708	0.152833250	0.749419927
0.846586021	0.346823289	0.749685029
0.652840531	-0.000143086	0.749736517
0.499884774	0.153127894	0.749656393
0.346645360	0.846873620	0.749636957
0.152869084	0.499785959	0.749607139
-0.000048395	0.652969861	0.749650584
0.846306936	0.846703940	0.749729958
0.652927651	0.499955445	0.749940167
0.499836410	0.653013021	0.749874221
0.319032409	0.486615245	0.915651243
0.165489753	0.179607179	0.915040584
0.012409216	0.332635737	0.915858235

0.819541048	0.486262197	0.916001057
0.666603165	0.180057332	0.916112184
0.513084007	0.332733762	0.916375467
0.319110864	0.986234678	0.916001856
0.166371970	0.679860095	0.916018426
0.012021117	0.831921212	0.915496954
0.819210468	0.986228518	0.916282539
0.665891770	0.679869317	0.916697784
0.513362088	0.833753832	0.915848329
0.165767464	0.333004411	0.020166609
0.666363680	0.333197706	0.020844358
0.165859706	0.832546818	0.020292955
0.665230663	0.832957642	0.021680463
0.001297260	0.000157129	0.145498344
0.497750867	0.000266083	0.146507583
0.000424834	0.500639759	0.146031267
0.499245134	0.495708496	0.145505177
0.334368354	0.171338510	0.187353347
0.832988743	0.166285348	0.187068877
0.335768023	0.666592152	0.186566770
0.831763666	0.666510203	0.187682230
0.167153434	0.333799103	0.312268326
0.667521244	0.333608903	0.313054283
0.167917978	0.833857552	0.311436745
0.667407598	0.834296027	0.312941741
0.000748830	0.000802647	0.353311616
0.499571759	-0.000130019	0.353576467
0.000584717	0.500675755	0.353569016
0.502068884	0.500758526	0.352203762
0.333787208	0.167361146	0.478668831
0.833526698	0.166925322	0.479284747
0.333909754	0.666642626	0.479137125
0.834093667	0.667495921	0.479315296
0.166916067	0.333506703	0.520117714
0.666927809	0.333844947	0.520596996
0.167102349	0.833538574	0.520005143
0.666859987	0.833468069	0.520373813
-0.000023721	0.000052468	0.645834454
0.499987509	0.000042939	0.645922739
0.000211492	0.500100815	0.645971878
0.500040909	0.500138887	0.646164499
0.333140242	0.166494123	0.686970345
0.833053891	0.166593340	0.687175194
0.333229973	0.666653703	0.687205478

0.833222480	0.666623106	0.687288440
0.166292806	0.332843255	0.812558820
0.666397286	0.333273122	0.812945676
0.166378767	0.833219818	0.812825916
0.666097924	0.833178263	0.813134553
-0.000950719	-0.000850092	0.853755056
0.499372058	0.000148507	0.853956646
-0.000198761	0.499834191	0.853891340
0.499450589	0.499438127	0.854484570
0.331195873	0.166041290	0.980561503
0.832681808	0.166096419	0.979512332
0.333766795	0.666960607	0.979614014
0.832480856	0.665961960	0.979881298

Interpolating coordinate: 0.450 (-823.099 eV)

0.175903434	0.009552610	0.081079614
0.328355150	0.316075607	0.079828967
0.486578113	0.167005168	0.083024011
0.679426381	0.014168311	0.083334700
0.833665706	0.319989082	0.083065890
0.985061886	0.165795361	0.082724780
0.179505133	0.513312249	0.082892981
0.332482847	0.820573988	0.082976268
0.484617922	0.670258977	0.082608465
0.683070382	0.513850858	0.082961540
0.832597560	0.819577978	0.083367743
0.986524909	0.666320677	0.083054838
0.150639962	0.152985985	0.250121956
-0.000255025	0.346868815	0.249993270
0.348377454	-0.002674614	0.250378526
0.653793722	0.153430690	0.250255940
0.503886883	0.349098476	0.253527069
0.846884098	0.000603930	0.250138260
0.153888772	0.652772712	0.249811133
0.000618712	0.847247646	0.249787825
0.346778949	0.499928733	0.250162443
0.657735984	0.657420301	0.252394187
0.500682367	0.846522042	0.250261305
0.848082286	0.500857453	0.250379299
0.013769873	0.180564701	0.417086230
0.320214601	0.334101889	0.416764053
0.166717165	0.486802968	0.416965036
0.514262228	0.180006617	0.417661030
0.820857534	0.334059757	0.417235631

0.667743305	0.487066990	0.417930508
0.014026378	0.680590281	0.416772515
0.319866013	0.833114923	0.417190812
0.167339915	0.986900299	0.416427340
0.514124540	0.680514664	0.417106496
0.821317743	0.835014407	0.417780660
0.666799896	0.986939251	0.417195525
0.486486249	0.319910573	0.583461568
0.180288187	0.166725636	0.583144363
0.333371124	0.013646667	0.583251268
0.986711366	0.319916384	0.583416904
0.680387119	0.166975840	0.583584159
0.833255766	0.013746813	0.583520511
0.486596155	0.819809344	0.583491151
0.180379492	0.666824702	0.583370958
0.333328395	0.513565692	0.583450011
0.986920057	0.819957099	0.583403580
0.680419124	0.666974562	0.583664296
0.833587900	0.513870771	0.583672301
0.346722059	0.346749028	0.749635880
0.152806629	-0.000352910	0.749440492
-0.000311771	0.152833993	0.749420757
0.846578919	0.346819843	0.749683386
0.652838464	-0.000144840	0.749737604
0.499878057	0.153120255	0.749652388
0.346644984	0.846872346	0.749639466
0.152861422	0.499786616	0.749601664
-0.000052412	0.652969368	0.749648217
0.846308114	0.846708706	0.749726964
0.652921896	0.499953270	0.749935554
0.499838405	0.653016006	0.749867850
0.319025512	0.486642672	0.915623790
0.165501970	0.179628029	0.915049203
0.012402387	0.332640010	0.915853766
0.819528078	0.486261216	0.916000372
0.666599146	0.180052558	0.916105508
0.513075984	0.332723466	0.916366797
0.319107745	0.986235744	0.916003143
0.166368576	0.679856380	0.916012627
0.012006328	0.831905017	0.915476596
0.819206446	0.986223332	0.916282825
0.665886800	0.679866077	0.916687650
0.513356335	0.833739533	0.915862747
0.165763854	0.333026684	0.020148371

0.666335329	0.333178650	0.020835142
0.165854266	0.832544094	0.020284617
0.665239067	0.832957311	0.021679175
0.001319249	0.000178488	0.145484106
0.497725501	0.000276268	0.146516963
0.000406691	0.500624197	0.146027815
0.499198108	0.495683329	0.145530729
0.334323864	0.171315451	0.187379023
0.832972863	0.166270414	0.187064736
0.335743217	0.666602177	0.186576381
0.831787212	0.666533560	0.187668335
0.167130610	0.333782236	0.312259475
0.667521612	0.333633319	0.313034603
0.167933415	0.833859501	0.311436322
0.667406765	0.834295438	0.312932590
0.000752561	0.000810741	0.353296366
0.499557094	-0.000138598	0.353571385
0.000583070	0.500676638	0.353569336
0.502077189	0.500759472	0.352241021
0.333786980	0.167355257	0.478658986
0.833519631	0.166925258	0.479277551
0.333907936	0.666634732	0.479140424
0.834112063	0.667512012	0.479317369
0.166908378	0.333499674	0.520112623
0.666933202	0.333853125	0.520587889
0.167110335	0.833537479	0.520001717
0.666863392	0.833474409	0.520365881
-0.000025009	0.000052862	0.645831072
0.499989375	0.000043576	0.645919870
0.000210749	0.500100733	0.645969719
0.500043662	0.500141744	0.646156397
0.333140423	0.166497131	0.686962782
0.833051866	0.166592798	0.687171424
0.333229364	0.666655071	0.687203488
0.833219072	0.666623897	0.687285628
0.166293396	0.332851075	0.812550715
0.666382403	0.333263808	0.812940068
0.166374623	0.833223587	0.812819982
0.666098585	0.833175127	0.813129191
-0.000939594	-0.000833702	0.853755883
0.499362269	0.000138365	0.853959042
-0.000213674	0.499831231	0.853885361
0.499443163	0.499429304	0.854474423
0.331196934	0.166039252	0.980599361

0.832673723	0.166095550	0.979511563
0.333746027	0.666949572	0.979608706
0.832476536	0.665968789	0.979865382

Interpolating coordinate: 0.467 (-823.052 eV)

0.175843203	0.009540246	0.081013093
0.328525134	0.316350815	0.079783754
0.486573367	0.166996165	0.083008541
0.679416081	0.014150443	0.083332916
0.833648078	0.319987293	0.083056691
0.985075780	0.165816832	0.082714678
0.179503754	0.513326671	0.082883382
0.332497339	0.820536910	0.082963506
0.484660588	0.670137124	0.082632652
0.682984660	0.513839613	0.082956370
0.832599357	0.819576776	0.083353035
0.986494031	0.666303767	0.083042273
0.150557024	0.152975660	0.250117638
-0.000269514	0.346867576	0.249984873
0.348423513	-0.002794368	0.250402749
0.653797119	0.153447937	0.250245154
0.504062375	0.349376331	0.253479917
0.846856774	0.000587284	0.250124798
0.153880410	0.652755525	0.249810458
0.000624369	0.847247767	0.249774215
0.346780266	0.499923359	0.250148182
0.657678540	0.657409353	0.252326953
0.500699386	0.846486108	0.250248429
0.848098490	0.500882093	0.250368849
0.013764292	0.180565106	0.417085763
0.320213071	0.334093689	0.416754469
0.166718382	0.486800009	0.416959554
0.514261831	0.180036750	0.417632327
0.820857863	0.334066291	0.417230933
0.667762089	0.487089727	0.417938626
0.014031039	0.680586611	0.416775700
0.319867681	0.833104106	0.417206944
0.167341498	0.986898608	0.416418021
0.514128143	0.680517477	0.417107407
0.821311086	0.834999397	0.417760135
0.666804375	0.986938422	0.417187993
0.486488295	0.319911364	0.583455045
0.180286998	0.166723860	0.583140519
0.333376966	0.013650867	0.583245270

0.986709126	0.319915728	0.583415541
0.680382009	0.166976391	0.583577074
0.833256840	0.013748273	0.583516690
0.486602418	0.819810024	0.583492975
0.180382340	0.666824109	0.583374997
0.333325396	0.513559620	0.583445824
0.986926958	0.819962474	0.583401922
0.680424746	0.666982118	0.583662620
0.833589007	0.513872445	0.583674322
0.346719217	0.346750618	0.749628965
0.152808820	-0.000345863	0.749439369
-0.000313833	0.152834736	0.749421588
0.846571817	0.346816396	0.749681743
0.652836398	-0.000146593	0.749738691
0.499871339	0.153112617	0.749648384
0.346644609	0.846871073	0.749641976
0.152853759	0.499787272	0.749596188
-0.000056429	0.652968875	0.749645850
0.846309292	0.846713473	0.749723970
0.652916140	0.499951095	0.749930941
0.499840400	0.653018991	0.749861480
0.319018616	0.486670098	0.915596336
0.165514188	0.179648879	0.915057821
0.012395559	0.332644283	0.915849296
0.819515108	0.486260235	0.915999688
0.666595127	0.180047785	0.916098833
0.513067960	0.332713171	0.916358127
0.319104627	0.986236810	0.916004430
0.166365182	0.679852665	0.916006828
0.011991538	0.831888821	0.915456237
0.819202424	0.986218146	0.916283111
0.665881830	0.679862838	0.916677516
0.513350581	0.833725234	0.915877164
0.165760243	0.333048957	0.020130132
0.666306977	0.333159594	0.020825925
0.165848826	0.832541370	0.020276279
0.665247472	0.832956980	0.021677886
0.001341239	0.000199848	0.145469868
0.497700136	0.000286452	0.146526343
0.000388548	0.500608636	0.146024363
0.499151082	0.495658162	0.145556282
0.334279374	0.171292392	0.187404699
0.832956982	0.166255479	0.187060595
0.335718411	0.666612202	0.186585992

0.831810757	0.666556917	0.187654440
0.167107786	0.333765370	0.312250625
0.667521980	0.333657735	0.313014924
0.167948852	0.833861449	0.311435899
0.667405932	0.834294848	0.312923440
0.000756292	0.000818835	0.353281117
0.499542429	-0.000147177	0.353566302
0.000581423	0.500677521	0.353569657
0.502085494	0.500760418	0.352278279
0.333786752	0.167349368	0.478649142
0.833512564	0.166925194	0.479270356
0.333906118	0.666626838	0.479143724
0.834130459	0.667528103	0.479319442
0.166900689	0.333492645	0.520107532
0.666938594	0.333861304	0.520578782
0.167118320	0.833536384	0.519998290
0.666866798	0.833480749	0.520357949
-0.000026296	0.000053256	0.645827690
0.499991241	0.000044213	0.645917001
0.000210006	0.500100651	0.645967560
0.500046414	0.500144602	0.646148295
0.333140605	0.166500138	0.686955220
0.833049841	0.166592256	0.687167655
0.333228755	0.666656439	0.687201499
0.833215664	0.666624687	0.687282816
0.166293986	0.332858895	0.812542610
0.666367521	0.333254495	0.812934461
0.166370478	0.833227357	0.812814047
0.666099246	0.833171990	0.813123830
-0.000928469	-0.000817312	0.853756711
0.499352481	0.000128223	0.853961438
-0.000228586	0.499828270	0.853879381
0.499435737	0.499420481	0.854464275
0.331197994	0.166037213	0.980637220
0.832665639	0.166094682	0.979510794
0.333725260	0.666938537	0.979603399
0.832472216	0.665975618	0.979849465

Interpolating coordinate: 0.483 (-823.060 eV)

0.175782973	0.009527881	0.080946572
0.328695118	0.316626023	0.079738540
0.486568622	0.166987161	0.082993071
0.679405780	0.014132576	0.083331131
0.833630449	0.319985504	0.083047491

0.985089674	0.165838303	0.082704577
0.179502374	0.513341093	0.082873782
0.332511832	0.820499833	0.082950744
0.484703255	0.670015272	0.082656839
0.682898938	0.513828368	0.082951199
0.832601155	0.819575574	0.083338326
0.986463153	0.666286857	0.083029707
0.150474085	0.152965334	0.250113319
-0.000284003	0.346866336	0.249976477
0.348469573	-0.002914123	0.250426973
0.653800515	0.153465184	0.250234367
0.504237868	0.349654187	0.253432764
0.846829449	0.000570639	0.250111336
0.153872047	0.652738338	0.249809784
0.000630026	0.847247889	0.249760604
0.346781582	0.499917985	0.250133922
0.657621095	0.657398405	0.252259719
0.500716405	0.846450173	0.250235554
0.848114693	0.500906734	0.250358399
0.013758711	0.180565510	0.417085297
0.320211541	0.334085490	0.416744886
0.166719600	0.486797049	0.416954071
0.514261435	0.180066882	0.417603625
0.820858193	0.334072824	0.417226235
0.667780872	0.487112463	0.417946743
0.014035699	0.680582941	0.416778884
0.319869350	0.833093289	0.417223075
0.167343082	0.986896917	0.416408701
0.514131746	0.680520289	0.417108317
0.821304429	0.834984388	0.417739610
0.666808854	0.986937592	0.417180462
0.486490341	0.319912156	0.583448521
0.180285808	0.166722084	0.583136675
0.333382807	0.013655067	0.583239273
0.986706887	0.319915073	0.583414177
0.680376900	0.166976943	0.583569989
0.833257914	0.013749733	0.583512870
0.486608680	0.819810703	0.583494800
0.180385189	0.666823515	0.583379037
0.333322396	0.513553547	0.583441638
0.986933858	0.819967849	0.583400263
0.680430367	0.666989674	0.583660944
0.833590114	0.513874119	0.583676344
0.346716376	0.346752209	0.749622049

0.152811012	-0.000338817	0.749438247
-0.000315896	0.152835479	0.749422418
0.846564715	0.346812950	0.749680099
0.652834331	-0.000148347	0.749739778
0.499864622	0.153104978	0.749644379
0.346644233	0.846869799	0.749644485
0.152846097	0.499787929	0.749590712
-0.000060447	0.652968383	0.749643483
0.846310469	0.846718239	0.749720976
0.652910385	0.499948920	0.749926328
0.499842396	0.653021976	0.749855109
0.319011719	0.486697525	0.915568883
0.165526405	0.179669730	0.915066440
0.012388730	0.332648557	0.915844827
0.819502138	0.486259254	0.915999003
0.666591108	0.180043011	0.916092157
0.513059937	0.332702875	0.916349457
0.319101509	0.986237875	0.916005717
0.166361788	0.679848949	0.916001028
0.011976749	0.831872626	0.915435879
0.819198402	0.986212961	0.916283396
0.665876861	0.679859598	0.916667382
0.513344828	0.833710935	0.915891582
0.165756633	0.333071229	0.020111894
0.666278626	0.333140538	0.020816709
0.165843386	0.832538645	0.020267941
0.665255876	0.832956649	0.021676597
0.001363228	0.000221207	0.145455630
0.497674770	0.000296637	0.146535722
0.000370405	0.500593074	0.146020911
0.499104055	0.495632995	0.145581834
0.334234884	0.171269334	0.187430374
0.832941102	0.166240545	0.187056454
0.335693605	0.666622227	0.186595602
0.831834302	0.666580273	0.187640546
0.167084963	0.333748503	0.312241774
0.667522348	0.333682151	0.312995244
0.167964289	0.833863398	0.311435476
0.667405099	0.834294259	0.312914289
0.000760023	0.000826928	0.353265867
0.499527763	-0.000155755	0.353561220
0.000579776	0.500678403	0.353569977
0.502093799	0.500761364	0.352315538
0.333786525	0.167343479	0.478639298

0.833505497	0.166925129	0.479263160
0.333904300	0.666618944	0.479147023
0.834148855	0.667544194	0.479321515
0.166893001	0.333485617	0.520102441
0.666943987	0.333869482	0.520569675
0.167126306	0.833535289	0.519994864
0.666870203	0.833487089	0.520350017
-0.000027584	0.000053650	0.645824308
0.499993106	0.000044850	0.645914132
0.000209264	0.500100569	0.645965401
0.500049167	0.500147459	0.646140193
0.333140786	0.166503146	0.686947657
0.833047816	0.166591714	0.687163885
0.333228146	0.666657807	0.687199509
0.833212256	0.666625478	0.687280004
0.166294577	0.332866715	0.812534504
0.666352639	0.333245181	0.812928853
0.166366334	0.833231126	0.812808113
0.666099907	0.833168854	0.813118468
-0.000917344	-0.000800922	0.853757538
0.499342692	0.000118080	0.853963834
-0.000243499	0.499825310	0.853873402
0.499428311	0.499411657	0.854454127
0.331199055	0.166035175	0.980675078
0.832657554	0.166093813	0.979510026
0.333704492	0.666927502	0.979598091
0.832467896	0.665982448	0.979833549

Interpolating coordinate: 0.500 (-823.055 eV)

0.175722742	0.009515516	0.080880051
0.328865102	0.316901231	0.079693327
0.486563877	0.166978158	0.082977601
0.679395480	0.014114708	0.083329346
0.833612821	0.319983715	0.083038292
0.985103568	0.165859774	0.082694475
0.179500995	0.513355515	0.082864183
0.332526324	0.820462755	0.082937982
0.484745921	0.669893420	0.082681026
0.682813215	0.513817123	0.082946029
0.832602952	0.819574372	0.083323617
0.986432275	0.666269947	0.083017141
0.150391147	0.152955009	0.250109001
-0.000298492	0.346865096	0.249968080
0.348515632	-0.003033878	0.250451196

0.653803911	0.153482431	0.250223581
0.504413361	0.349932043	0.253385612
0.846802125	0.000553993	0.250097874
0.153863685	0.652721151	0.249809110
0.000635683	0.847248010	0.249746994
0.346782899	0.499912611	0.250119662
0.657563651	0.657387457	0.252192486
0.500733424	0.846414239	0.250222678
0.848130897	0.500931374	0.250347949
0.013753130	0.180565915	0.417084831
0.320210012	0.334077290	0.416735302
0.166720817	0.486794090	0.416948588
0.514261038	0.180097014	0.417574922
0.820858522	0.334079358	0.417221536
0.667799656	0.487135199	0.417954860
0.014040360	0.680579271	0.416782068
0.319871018	0.833082472	0.417239207
0.167344666	0.986895226	0.416399382
0.514135349	0.680523102	0.417109228
0.821297773	0.834969379	0.417719085
0.666813333	0.986936762	0.417172930
0.486492387	0.319912948	0.583441998
0.180284619	0.166720308	0.583132830
0.333388649	0.013659267	0.583233275
0.986704648	0.319914417	0.583412813
0.680371791	0.166977494	0.583562904
0.833258988	0.013751192	0.583509049
0.486614942	0.819811383	0.583496625
0.180388038	0.666822921	0.583383076
0.333319397	0.513547475	0.583437451
0.986940759	0.819973224	0.583398605
0.680435988	0.666997230	0.583659268
0.833591221	0.513875793	0.583678365
0.346713535	0.346753799	0.749615134
0.152813204	-0.000331770	0.749437124
-0.000317959	0.152836222	0.749423248
0.846557613	0.346809504	0.749678456
0.652832265	-0.000150101	0.749740865
0.499857905	0.153097339	0.749640374
0.346643858	0.846868526	0.749646994
0.152838434	0.499788585	0.749585237
-0.000064464	0.652967890	0.749641116
0.846311647	0.846723006	0.749717982
0.652904629	0.499946745	0.749921715

0.499844391	0.653024961	0.749848738
0.319004823	0.486724951	0.915541430
0.165538622	0.179690580	0.915075059
0.012381902	0.332652830	0.915840357
0.819489168	0.486258273	0.915998319
0.666587089	0.180038238	0.916085482
0.513051914	0.332692580	0.916340787
0.319098390	0.986238941	0.916007004
0.166358394	0.679845234	0.915995229
0.011961959	0.831856431	0.915415520
0.819194380	0.986207775	0.916283682
0.665871891	0.679856358	0.916657248
0.513339075	0.833696636	0.915905999
0.165753022	0.333093502	0.020093655
0.666250275	0.333121482	0.020807492
0.165837946	0.832535921	0.020259603
0.665264281	0.832956318	0.021675309
0.001385218	0.000242567	0.145441392
0.497649405	0.000306821	0.146545102
0.000352262	0.500577512	0.146017459
0.499057029	0.495607828	0.145607386
0.334190394	0.171246275	0.187456050
0.832925221	0.166225611	0.187052313
0.335668799	0.666632252	0.186605213
0.831857848	0.666603630	0.187626651
0.167062139	0.333731636	0.312232923
0.667522716	0.333706567	0.312975564
0.167979726	0.833865346	0.311435053
0.667404266	0.834293669	0.312905139
0.000763754	0.000835022	0.353250617
0.499513098	-0.000164334	0.353556137
0.000578129	0.500679286	0.353570298
0.502102104	0.500762310	0.352352796
0.333786297	0.167337590	0.478629453
0.833498430	0.166925065	0.479255964
0.333902482	0.666611050	0.479150323
0.834167251	0.667560285	0.479323588
0.166885312	0.333478588	0.520097350
0.666949380	0.333877661	0.520560568
0.167134292	0.833534194	0.519991437
0.666873608	0.833493429	0.520342085
-0.000028872	0.000054044	0.645820926
0.499994972	0.000045487	0.645911263
0.000208521	0.500100487	0.645963242

0.500051919	0.500150317	0.646132091
0.333140968	0.166506153	0.686940095
0.833045791	0.166591172	0.687160115
0.333227537	0.666659175	0.687197519
0.833208848	0.666626268	0.687277192
0.166295167	0.332874535	0.812526399
0.666337756	0.333235868	0.812923246
0.166362189	0.833234895	0.812802178
0.666100568	0.833165717	0.813113107
-0.000906219	-0.000784532	0.853758365
0.499332904	0.000107938	0.853966230
-0.000258412	0.499822350	0.853867423
0.499420885	0.499402834	0.854443980
0.331200115	0.166033136	0.980712937
0.832649470	0.166092944	0.979509257
0.333683725	0.666916467	0.979592784
0.832463576	0.665989277	0.979817632

Interpolating coordinate: 0.517 (-823.056 eV)

0.175662511	0.009503151	0.080813530
0.329035086	0.317176439	0.079648114
0.486559132	0.166969155	0.082962131
0.679385180	0.014096841	0.083327561
0.833595193	0.319981926	0.083029093
0.985117462	0.165881245	0.082684373
0.179499616	0.513369937	0.082854584
0.332540816	0.820425677	0.082925220
0.484788587	0.669771568	0.082705213
0.682727492	0.513805878	0.082940859
0.832604749	0.819573170	0.083308908
0.986401397	0.666253037	0.083004575
0.150308209	0.152944684	0.250104683
-0.000312981	0.346863856	0.249959684
0.348561691	-0.003153633	0.250475419
0.653807307	0.153499678	0.250212795
0.504588854	0.350209899	0.253338460
0.846774801	0.000537347	0.250084412
0.153855323	0.652703964	0.249808436
0.000641340	0.847248131	0.249733384
0.346784216	0.499907237	0.250105402
0.657506207	0.657376509	0.252125253
0.500750443	0.846378305	0.250209802
0.848147101	0.500956015	0.250337499
0.013747549	0.180566320	0.417084365

0.320208483	0.334069090	0.416725718
0.166722034	0.486791131	0.416943105
0.514260641	0.180127146	0.417546219
0.820858851	0.334085891	0.417216837
0.667818440	0.487157935	0.417962977
0.014045021	0.680575601	0.416785252
0.319872687	0.833071655	0.417255339
0.167346250	0.986893535	0.416390063
0.514138952	0.680525915	0.417110139
0.821291116	0.834954370	0.417698560
0.666817812	0.986935932	0.417165398
0.486494433	0.319913740	0.583435475
0.180283430	0.166718532	0.583128985
0.333394491	0.013663467	0.583227278
0.986702409	0.319913761	0.583411449
0.680366682	0.166978045	0.583555819
0.833260062	0.013752651	0.583505228
0.486621204	0.819812063	0.583498450
0.180390887	0.666822327	0.583387115
0.333316398	0.513541403	0.583433264
0.986947660	0.819978599	0.583396947
0.680441609	0.667004786	0.583657592
0.833592328	0.513877467	0.583680386
0.346710694	0.346755389	0.749608219
0.152815396	-0.000324723	0.749436001
-0.000320022	0.152836965	0.749424078
0.846550511	0.346806058	0.749676813
0.652830199	-0.000151855	0.749741952
0.499851188	0.153089700	0.749636369
0.346643483	0.846867252	0.749649503
0.152830771	0.499789241	0.749579762
-0.000068481	0.652967397	0.749638749
0.846312825	0.846727773	0.749714988
0.652898873	0.499944570	0.749917102
0.499846386	0.653027946	0.749842367
0.318997926	0.486752377	0.915513977
0.165550839	0.179711430	0.915083678
0.012375074	0.332657103	0.915835887
0.819476198	0.486257292	0.915997634
0.666583070	0.180033464	0.916078806
0.513043891	0.332682285	0.916332117
0.319095271	0.986240007	0.916008291
0.166355000	0.679841519	0.915989430
0.011947170	0.831840236	0.915395161

0.819190358	0.986202589	0.916283968
0.665866921	0.679853118	0.916647114
0.513333322	0.833682337	0.915920417
0.165749411	0.333115775	0.020075416
0.666221924	0.333102426	0.020798276
0.165832506	0.832533197	0.020251265
0.665272686	0.832955987	0.021674021
0.001407207	0.000263927	0.145427154
0.497624040	0.000317005	0.146554482
0.000334119	0.500561950	0.146014007
0.499010003	0.495582661	0.145632938
0.334145904	0.171223216	0.187481726
0.832909340	0.166210677	0.187048172
0.335643993	0.666642277	0.186614824
0.831881393	0.666626987	0.187612756
0.167039315	0.333714769	0.312224072
0.667523084	0.333730983	0.312955884
0.167995163	0.833867294	0.311434630
0.667403433	0.834293079	0.312895989
0.000767485	0.000843116	0.353235367
0.499498433	-0.000172913	0.353551054
0.000576482	0.500680169	0.353570619
0.502110409	0.500763256	0.352390055
0.333786069	0.167331701	0.478619608
0.833491363	0.166925001	0.479248768
0.333900664	0.666603156	0.479153622
0.834185647	0.667576376	0.479325661
0.166877623	0.333471559	0.520092259
0.666954773	0.333885840	0.520551461
0.167142278	0.833533099	0.519988010
0.666877013	0.833499769	0.520334153
-0.000030160	0.000054438	0.645817544
0.499996838	0.000046124	0.645908394
0.000207778	0.500100405	0.645961083
0.500054671	0.500153175	0.646123989
0.333141150	0.166509160	0.686932533
0.833043766	0.166590630	0.687156345
0.333226928	0.666660543	0.687195529
0.833205440	0.666627059	0.687274380
0.166295757	0.332882355	0.812518294
0.666322873	0.333226554	0.812917639
0.166358044	0.833238664	0.812796243
0.666101229	0.833162581	0.813107745
-0.000895094	-0.000768142	0.853759192

0.499323116	0.000097796	0.853968626
-0.000273325	0.499819390	0.853861444
0.499413459	0.499394011	0.854433833
0.331201176	0.166031097	0.980750796
0.832641385	0.166092075	0.979508488
0.333662958	0.666905432	0.979587476
0.832459256	0.665996106	0.979801715

Interpolating coordinate: 0.533 (-823.053 eV)

0.175602281	0.009490787	0.080747009
0.329205070	0.317451647	0.079602901
0.486554387	0.166960151	0.082946661
0.679374879	0.014078973	0.083325776
0.833577564	0.319980137	0.083019893
0.985131356	0.165902716	0.082674272
0.179498236	0.513384359	0.082844984
0.332555309	0.820388600	0.082912458
0.484831254	0.669649716	0.082729400
0.682641770	0.513794633	0.082935689
0.832606547	0.819571968	0.083294199
0.986370519	0.666236127	0.082992009
0.150225270	0.152934358	0.250100364
-0.000327470	0.346862616	0.249951287
0.348607751	-0.003273388	0.250499643
0.653810703	0.153516925	0.250202008
0.504764346	0.350487755	0.253291307
0.846747476	0.000520702	0.250070950
0.153846960	0.652686777	0.249807762
0.000646997	0.847248253	0.249719773
0.346785532	0.499901863	0.250091142
0.657448763	0.657365561	0.252058019
0.500767462	0.846342370	0.250196927
0.848163304	0.500980655	0.250327049
0.013741968	0.180566724	0.417083898
0.320206953	0.334060891	0.416716135
0.166723252	0.486788171	0.416937623
0.514260245	0.180157278	0.417517517
0.820859181	0.334092425	0.417212139
0.667837223	0.487180672	0.417971095
0.014049681	0.680571931	0.416788436
0.319874355	0.833060838	0.417271471
0.167347834	0.986891844	0.416380744
0.514142555	0.680528727	0.417111049
0.821284460	0.834939361	0.417678035

0.666822291	0.986935103	0.417157867
0.486496479	0.319914532	0.583428951
0.180282240	0.166716756	0.583125141
0.333400332	0.013667667	0.583221280
0.986700169	0.319913106	0.583410086
0.680361573	0.166978597	0.583548734
0.833261136	0.013754111	0.583501408
0.486627466	0.819812743	0.583500275
0.180393736	0.666821733	0.583391155
0.333313398	0.513535330	0.583429078
0.986954560	0.819983974	0.583395289
0.680447230	0.667012342	0.583655916
0.833593435	0.513879141	0.583682408
0.346707852	0.346756980	0.749601304
0.152817588	-0.000317677	0.749434879
-0.000322084	0.152837708	0.749424908
0.846543409	0.346802612	0.749675169
0.652828132	-0.000153608	0.749743039
0.499844470	0.153082061	0.749632364
0.346643107	0.846865979	0.749652012
0.152823109	0.499789898	0.749574286
-0.000072499	0.652966905	0.749636382
0.846314002	0.846732539	0.749711994
0.652893118	0.499942395	0.749912489
0.499848382	0.653030931	0.749835996
0.318991030	0.486779804	0.915486524
0.165563057	0.179732281	0.915092297
0.012368245	0.332661377	0.915831418
0.819463228	0.486256311	0.915996950
0.666579051	0.180028691	0.916072131
0.513035868	0.332671989	0.916323447
0.319092153	0.986241072	0.916009578
0.166351606	0.679837804	0.915983630
0.011932380	0.831824040	0.915374803
0.819186336	0.986197404	0.916284254
0.665861952	0.679849878	0.916636980
0.513327569	0.833668038	0.915934834
0.165745801	0.333138047	0.020057178
0.666193573	0.333083370	0.020789059
0.165827066	0.832530472	0.020242927
0.665281090	0.832955656	0.021672732
0.001429197	0.000285286	0.145412916
0.497598674	0.000327190	0.146563862
0.000315976	0.500546388	0.146010555

0.498962976	0.495557494	0.145658491
0.334101414	0.171200157	0.187507401
0.832893460	0.166195743	0.187044031
0.335619187	0.666652302	0.186624434
0.831904939	0.666650343	0.187598862
0.167016492	0.333697902	0.312215222
0.667523452	0.333755399	0.312936204
0.168010600	0.833869243	0.311434207
0.667402600	0.834292490	0.312886838
0.000771216	0.000851209	0.353220117
0.499483768	-0.000181492	0.353545972
0.000574835	0.500681051	0.353570939
0.502118714	0.500764202	0.352427313
0.333785842	0.167325812	0.478609764
0.833484296	0.166924936	0.479241572
0.333898846	0.666595262	0.479156922
0.834204043	0.667592467	0.479327734
0.166869935	0.333464530	0.520087168
0.666960165	0.333894018	0.520542354
0.167150264	0.833532004	0.519984584
0.666880419	0.833506109	0.520326221
-0.000031448	0.000054832	0.645814162
0.499998703	0.000046761	0.645905525
0.000207036	0.500100323	0.645958924
0.500057424	0.500156032	0.646115887
0.333141331	0.166512168	0.686924970
0.833041741	0.166590088	0.687152576
0.333226319	0.666661911	0.687193540
0.833202032	0.666627849	0.687271568
0.166296348	0.332890175	0.812510188
0.666307991	0.333217241	0.812912031
0.166353900	0.833242433	0.812790309
0.666101890	0.833159444	0.813102384
-0.000883969	-0.000751752	0.853760019
0.499313327	0.000087653	0.853971022
-0.000288238	0.499816430	0.853855465
0.499406033	0.499385187	0.854423685
0.331202236	0.166029059	0.980788654
0.832633301	0.166091207	0.979507720
0.333642190	0.666894397	0.979582169
0.832454936	0.666002936	0.979785799

Interpolating coordinate: 0.550 (-823.099 eV)

0.175542050	0.009478422	0.080680489
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0.329375054	0.317726855	0.079557687
0.486549642	0.166951148	0.082931191
0.679364579	0.014061106	0.083323992
0.833559936	0.319978348	0.083010694
0.985145251	0.165924187	0.082664170
0.179496857	0.513398781	0.082835385
0.332569801	0.820351522	0.082899696
0.484873920	0.669527863	0.082753587
0.682556047	0.513783387	0.082930518
0.832608344	0.819570766	0.083279491
0.986339641	0.666219217	0.082979444
0.150142332	0.152924033	0.250096046
-0.000341959	0.346861376	0.249942891
0.348653810	-0.003393142	0.250523866
0.653814099	0.153534173	0.250191221
0.504939839	0.350765610	0.253244155
0.846720152	0.000504056	0.250057488
0.153838598	0.652669590	0.249807087
0.000652654	0.847248374	0.249706163
0.346786849	0.499896489	0.250076881
0.657391318	0.657354613	0.251990785
0.500784481	0.846306436	0.250184052
0.848179508	0.501005295	0.250316599
0.013736387	0.180567129	0.417083432
0.320205423	0.334052691	0.416706551
0.166724469	0.486785212	0.416932140
0.514259848	0.180187410	0.417488814
0.820859510	0.334098958	0.417207440
0.667856007	0.487203408	0.417979212
0.014054342	0.680568261	0.416791621
0.319876023	0.833050021	0.417287602
0.167349417	0.986890153	0.416371424
0.514146158	0.680531540	0.417111960
0.821277804	0.834924352	0.417657510
0.666826770	0.986934273	0.417150335
0.486498525	0.319915323	0.583422428
0.180281051	0.166714980	0.583121296
0.333406174	0.013671867	0.583215282
0.986697930	0.319912450	0.583408722
0.680356463	0.166979148	0.583541649
0.833262210	0.013755570	0.583497588
0.486633728	0.819813422	0.583502099
0.180396584	0.666821139	0.583395194
0.333310399	0.513529258	0.583424891

0.986961461	0.819989349	0.583393630
0.680452852	0.667019898	0.583654240
0.833594541	0.513880815	0.583684429
0.346705011	0.346758570	0.749594388
0.152819780	-0.000310630	0.749433756
-0.000324147	0.152838451	0.749425738
0.846536307	0.346799165	0.749673526
0.652826066	-0.000155362	0.749744126
0.499837753	0.153074422	0.749628360
0.346642732	0.846864705	0.749654521
0.152815446	0.499790554	0.749568811
-0.000076516	0.652966412	0.749634015
0.846315180	0.846737306	0.749709000
0.652887363	0.499940221	0.749907876
0.499850377	0.653033916	0.749829626
0.318984133	0.486807231	0.915459071
0.165575274	0.179753131	0.915100915
0.012361416	0.332665650	0.915826948
0.819450258	0.486255330	0.915996265
0.666575032	0.180023917	0.916065455
0.513027844	0.332661694	0.916314777
0.319089035	0.986242138	0.916010865
0.166348212	0.679834088	0.915977831
0.011917591	0.831807845	0.915354445
0.819182314	0.986192218	0.916284539
0.665856982	0.679846639	0.916626846
0.513321816	0.833653739	0.915949252
0.165742190	0.333160320	0.020038939
0.666165221	0.333064315	0.020779842
0.165821626	0.832527748	0.020234589
0.665289495	0.832955325	0.021671443
0.001451186	0.000306645	0.145398678
0.497573309	0.000337374	0.146573241
0.000297833	0.500530827	0.146007103
0.498915950	0.495532327	0.145684043
0.334056924	0.171177099	0.187533077
0.832877579	0.166180808	0.187039890
0.335594382	0.666662328	0.186634045
0.831928484	0.666673700	0.187584967
0.166993668	0.333681036	0.312206371
0.667523820	0.333779815	0.312916525
0.168026037	0.833871191	0.311433784
0.667401767	0.834291900	0.312877688
0.000774947	0.000859303	0.353204867

0.499469102	-0.000190070	0.353540889
0.000573188	0.500681934	0.353571260
0.502127019	0.500765148	0.352464571
0.333785614	0.167319923	0.478599919
0.833477229	0.166924872	0.479234377
0.333897028	0.666587368	0.479160221
0.834222439	0.667608557	0.479329807
0.166862246	0.333457502	0.520082077
0.666965558	0.333902196	0.520533247
0.167158249	0.833530909	0.519981157
0.666883824	0.833512449	0.520318289
-0.000032735	0.000055226	0.645810780
0.500000569	0.000047398	0.645902656
0.000206293	0.500100240	0.645956765
0.500060176	0.500158890	0.646107784
0.333141513	0.166515175	0.686917408
0.833039716	0.166589546	0.687148806
0.333225710	0.666663280	0.687191550
0.833198623	0.666628640	0.687268756
0.166296938	0.332897995	0.812502083
0.666293109	0.333207928	0.812906424
0.166349755	0.833246203	0.812784374
0.666102551	0.833156307	0.813097022
-0.000872844	-0.000735362	0.853760847
0.499303539	0.000077511	0.853973418
-0.000303150	0.499813469	0.853849485
0.499398607	0.499376364	0.854413537
0.331203297	0.166027020	0.980826513
0.832625216	0.166090338	0.979506951
0.333621423	0.666883362	0.979576862
0.832450616	0.666009765	0.979769882

Interpolating coordinate: 0.567 (-823.107 eV)

0.175481819	0.009466057	0.080613968
0.329545038	0.318002063	0.079512474
0.486544897	0.166942145	0.082915721
0.679354278	0.014043238	0.083322207
0.833542308	0.319976559	0.083001495
0.985159145	0.165945658	0.082654069
0.179495477	0.513413203	0.082825786
0.332584294	0.820314445	0.082886934
0.484916587	0.669406011	0.082777774
0.682470325	0.513772142	0.082925348
0.832610142	0.819569564	0.083264782

0.986308763	0.666202307	0.082966878
0.150059394	0.152913707	0.250091727
-0.000356448	0.346860136	0.249934494
0.348699870	-0.003512897	0.250548089
0.653817495	0.153551420	0.250180435
0.505115332	0.351043466	0.253197003
0.846692827	0.000487411	0.250044026
0.153830235	0.652652403	0.249806413
0.000658311	0.847248495	0.249692553
0.346788166	0.499891115	0.250062621
0.657333874	0.657343665	0.251923552
0.500801500	0.846270502	0.250171176
0.848195711	0.501029936	0.250306149
0.013730806	0.180567533	0.417082966
0.320203894	0.334044491	0.416696968
0.166725686	0.486782252	0.416926657
0.514259451	0.180217542	0.417460112
0.820859840	0.334105492	0.417202742
0.667874791	0.487226144	0.417987329
0.014059003	0.680564591	0.416794805
0.319877692	0.833039204	0.417303734
0.167351001	0.986888462	0.416362105
0.514149761	0.680534353	0.417112870
0.821271147	0.834909343	0.417636985
0.666831249	0.986933443	0.417142804
0.486500571	0.319916115	0.583415904
0.180279862	0.166713204	0.583117452
0.333412016	0.013676067	0.583209285
0.986695691	0.319911795	0.583407358
0.680351354	0.166979699	0.583534564
0.833263284	0.013757030	0.583493767
0.486639990	0.819814102	0.583503924
0.180399433	0.666820545	0.583399233
0.333307399	0.513523186	0.583420704
0.986968361	0.819994724	0.583391972
0.680458473	0.667027454	0.583652564
0.833595648	0.513882489	0.583686451
0.346702170	0.346760161	0.749587473
0.152821972	-0.000303584	0.749432633
-0.000326210	0.152839194	0.749426568
0.846529205	0.346795719	0.749671883
0.652823999	-0.000157116	0.749745213
0.499831036	0.153066783	0.749624355
0.346642356	0.846863432	0.749657030

0.152807784	0.499791211	0.749563335
-0.000080533	0.652965919	0.749631648
0.846316357	0.846742072	0.749706006
0.652881607	0.499938046	0.749903263
0.499852372	0.653036901	0.749823255
0.318977237	0.486834657	0.915431618
0.165587491	0.179773982	0.915109534
0.012354588	0.332669923	0.915822478
0.819437288	0.486254349	0.915995581
0.666571013	0.180019144	0.916058780
0.513019821	0.332651398	0.916306107
0.319085916	0.986243204	0.916012152
0.166344818	0.679830373	0.915972032
0.011902801	0.831791650	0.915334086
0.819178292	0.986187032	0.916284825
0.665852013	0.679843399	0.916616712
0.513316063	0.833639440	0.915963669
0.165738580	0.333182593	0.020020700
0.666136870	0.333045259	0.020770626
0.165816186	0.832525024	0.020226251
0.665297899	0.832954994	0.021670155
0.001473176	0.000328005	0.145384440
0.497547944	0.000347559	0.146582621
0.000279690	0.500515265	0.146003651
0.498868924	0.495507160	0.145709595
0.334012434	0.171154040	0.187558753
0.832861699	0.166165874	0.187035749
0.335569576	0.666672353	0.186643656
0.831952030	0.666697057	0.187571073
0.166970844	0.333664169	0.312197520
0.667524188	0.333804231	0.312896845
0.168041474	0.833873140	0.311433361
0.667400934	0.834291311	0.312868537
0.000778678	0.000867396	0.353189617
0.499454437	-0.000198649	0.353535806
0.000571541	0.500682816	0.353571580
0.502135324	0.500766094	0.352501830
0.333785387	0.167314034	0.478590075
0.833470162	0.166924808	0.479227181
0.333895210	0.666579474	0.479163521
0.834240835	0.667624648	0.479331880
0.166854557	0.333450473	0.520076986
0.666970951	0.333910375	0.520524140
0.167166235	0.833529814	0.519977730

0.666887229	0.833518789	0.520310357
-0.000034023	0.000055620	0.645807398
0.500002434	0.000048035	0.645899787
0.000205550	0.500100158	0.645954606
0.500062929	0.500161748	0.646099682
0.333141694	0.166518183	0.686909845
0.833037691	0.166589004	0.687145036
0.333225101	0.666664648	0.687189560
0.833195215	0.666629430	0.687265944
0.166297528	0.332905815	0.812493977
0.666278226	0.333198614	0.812900816
0.166345610	0.833249972	0.812778440
0.666103212	0.833153171	0.813091661
-0.000861719	-0.000718972	0.853761674
0.499293750	0.000067369	0.853975814
-0.000318063	0.499810509	0.853843506
0.499391181	0.499367541	0.854403390
0.331204357	0.166024982	0.980864372
0.832617132	0.166089469	0.979506182
0.333600655	0.666872327	0.979571554
0.832446296	0.666016595	0.979753966

Interpolating coordinate: 0.583 (-823.114 eV)

0.175421589	0.009453692	0.080547447
0.329715023	0.318277270	0.079467261
0.486540151	0.166933141	0.082900251
0.679343978	0.014025371	0.083320422
0.833524679	0.319974771	0.082992296
0.985173039	0.165967129	0.082643967
0.179494098	0.513427625	0.082816186
0.332598786	0.820277367	0.082874171
0.484959253	0.669284159	0.082801961
0.682384602	0.513760897	0.082920178
0.832611940	0.819568362	0.083250073
0.986277885	0.666185397	0.082954312
0.149976455	0.152903381	0.250087409
-0.000370937	0.346858897	0.249926097
0.348745929	-0.003632652	0.250572313
0.653820892	0.153568667	0.250169649
0.505290825	0.351321322	0.253149850
0.846665503	0.000470765	0.250030564
0.153821873	0.652635216	0.249805739
0.000663967	0.847248617	0.249678943
0.346789482	0.499885741	0.250048361

0.657276430	0.657332717	0.251856319
0.500818519	0.846234568	0.250158300
0.848211915	0.501054577	0.250295699
0.013725225	0.180567938	0.417082499
0.320202365	0.334036292	0.416687384
0.166726903	0.486779293	0.416921174
0.514259054	0.180247675	0.417431409
0.820860169	0.334112025	0.417198043
0.667893575	0.487248881	0.417995446
0.014063664	0.680560922	0.416797989
0.319879360	0.833028387	0.417319866
0.167352585	0.986886772	0.416352786
0.514153363	0.680537165	0.417113781
0.821264490	0.834894334	0.417616461
0.666835728	0.986932614	0.417135272
0.486502617	0.319916907	0.583409381
0.180278673	0.166711428	0.583113607
0.333417857	0.013680267	0.583203287
0.986693451	0.319911139	0.583405995
0.680346245	0.166980250	0.583527478
0.833264358	0.013758489	0.583489947
0.486646252	0.819814782	0.583505749
0.180402282	0.666819951	0.583403273
0.333304400	0.513517114	0.583416518
0.986975262	0.820000099	0.583390314
0.680464094	0.667035010	0.583650889
0.833596755	0.513884162	0.583688472
0.346699329	0.346761751	0.749580558
0.152824163	-0.000296537	0.749431511
-0.000328272	0.152839937	0.749427398
0.846522103	0.346792273	0.749670240
0.652821933	-0.000158870	0.749746299
0.499824318	0.153059144	0.749620350
0.346641981	0.846862159	0.749659540
0.152800121	0.499791867	0.749557860
-0.000084551	0.652965427	0.749629280
0.846317535	0.846746839	0.749703011
0.652875851	0.499935871	0.749898650
0.499854368	0.653039886	0.749816884
0.318970341	0.486862084	0.915404164
0.165599708	0.179794832	0.915118153
0.012347759	0.332674197	0.915818009
0.819424317	0.486253368	0.915994896
0.666566994	0.180014370	0.916052104

0.513011798	0.332641103	0.916297437
0.319082798	0.986244269	0.916013440
0.166341425	0.679826658	0.915966232
0.011888012	0.831775455	0.915313728
0.819174269	0.986181847	0.916285111
0.665847043	0.679840159	0.916606578
0.513310310	0.833625141	0.915978087
0.165734969	0.333204866	0.020002461
0.666108519	0.333026203	0.020761410
0.165810746	0.832522299	0.020217914
0.665306304	0.832954663	0.021668867
0.001495165	0.000349364	0.145370202
0.497522579	0.000357743	0.146592001
0.000261548	0.500499703	0.146000199
0.498821897	0.495481993	0.145735147
0.333967944	0.171130981	0.187584429
0.832845819	0.166150940	0.187031608
0.335544770	0.666682378	0.186653266
0.831975575	0.666720413	0.187557178
0.166948021	0.333647302	0.312188670
0.667524556	0.333828646	0.312877165
0.168056911	0.833875088	0.311432938
0.667400101	0.834290721	0.312859387
0.000782409	0.000875490	0.353174367
0.499439772	-0.000207228	0.353530724
0.000569894	0.500683699	0.353571901
0.502143629	0.500767040	0.352539089
0.333785159	0.167308145	0.478580230
0.833463095	0.166924744	0.479219985
0.333893392	0.666571580	0.479166821
0.834259231	0.667640739	0.479333954
0.166846869	0.333443444	0.520071895
0.666976344	0.333918553	0.520515033
0.167174221	0.833528719	0.519974303
0.666890634	0.833525130	0.520302425
-0.000035311	0.000056014	0.645804016
0.500004300	0.000048672	0.645896918
0.000204808	0.500100076	0.645952447
0.500065681	0.500164605	0.646091580
0.333141876	0.166521190	0.686902283
0.833035665	0.166588462	0.687141266
0.333224492	0.666666016	0.687187571
0.833191807	0.666630221	0.687263131
0.166298118	0.332913635	0.812485872

0.666263344	0.333189301	0.812895209
0.166341466	0.833253741	0.812772505
0.666103872	0.833150035	0.813086299
-0.000850593	-0.000702582	0.853762501
0.499283962	0.000057227	0.853978211
-0.000332976	0.499807549	0.853837527
0.499383755	0.499358718	0.854393243
0.331205417	0.166022943	0.980902230
0.832609047	0.166088601	0.979505414
0.333579888	0.666861292	0.979566247
0.832441975	0.666023424	0.979738049

Interpolating coordinate: 0.667 (-823.145 eV)

0.175120435	0.009391869	0.080214843
0.330564943	0.319653310	0.079241195
0.486516426	0.166888125	0.082822901
0.679292476	0.013936033	0.083311498
0.833436538	0.319965826	0.082946299
0.985242510	0.166074484	0.082593459
0.179487201	0.513499736	0.082768190
0.332671248	0.820091979	0.082810361
0.485172585	0.668674898	0.082922897
0.681955989	0.513704671	0.082894327
0.832620927	0.819562352	0.083176529
0.986123495	0.666100847	0.082891483
0.149561764	0.152851754	0.250065817
-0.000443383	0.346852697	0.249884115
0.348976226	-0.004231426	0.250693429
0.653837872	0.153654903	0.250115716
0.506168288	0.352710601	0.252914089
0.846528881	0.000387537	0.249963255
0.153780060	0.652549281	0.249802368
0.000692252	0.847249223	0.249610891
0.346796066	0.499858871	0.249977060
0.656989209	0.657277977	0.251520151
0.500903614	0.846054896	0.250093923
0.848292933	0.501177779	0.250243450
0.013697320	0.180569961	0.417080168
0.320194717	0.333995293	0.416639466
0.166732990	0.486764496	0.416893761
0.514257071	0.180398335	0.417287896
0.820861816	0.334144692	0.417174550
0.667987493	0.487362562	0.418036033
0.014086967	0.680542572	0.416813910

0.319887703	0.832974302	0.417400525
0.167360504	0.986878317	0.416306190
0.514171378	0.680551229	0.417118334
0.821231208	0.834819288	0.417513836
0.666858123	0.986928465	0.417097614
0.486512847	0.319920866	0.583376764
0.180272726	0.166702547	0.583094384
0.333447066	0.013701268	0.583173300
0.986682255	0.319907861	0.583399176
0.680320699	0.166983007	0.583492053
0.833269729	0.013765786	0.583470844
0.486677563	0.819818181	0.583514873
0.180416526	0.666816982	0.583423469
0.333289403	0.513486752	0.583395584
0.987009765	0.820026975	0.583382023
0.680492200	0.667072790	0.583642509
0.833602289	0.513892532	0.583698580
0.346685122	0.346769703	0.749545982
0.152835123	-0.000261304	0.749425897
-0.000338586	0.152843652	0.749431549
0.846486593	0.346775042	0.749662023
0.652811601	-0.000167638	0.749751734
0.499790732	0.153020950	0.749600326
0.346640104	0.846855791	0.749672085
0.152761808	0.499795149	0.749530482
-0.000104637	0.652962963	0.749617445
0.846323423	0.846770672	0.749688041
0.652847074	0.499924997	0.749875585
0.499864344	0.653054812	0.749785030
0.318935858	0.486999216	0.915266899
0.165660795	0.179899084	0.915161247
0.012313617	0.332695563	0.915795660
0.819359467	0.486248463	0.915991473
0.666546899	0.179990503	0.916018727
0.512971682	0.332589626	0.916254086
0.319067205	0.986249598	0.916019875
0.166324455	0.679808082	0.915937236
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0.819154159	0.986155918	0.916286540
0.665822195	0.679823960	0.916555909
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0.165716917	0.333316229	0.019911268
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0.000170833	0.500421894	0.145982939
0.498586766	0.495356157	0.145862909
0.333745493	0.171015687	0.187712807
0.832766416	0.166076269	0.187010903
0.335420741	0.666732504	0.186701320
0.832093302	0.666837197	0.187487705
0.166833902	0.333562968	0.312144416
0.667526395	0.333950726	0.312778766
0.168134096	0.833884831	0.311430823
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0.333142784	0.166536227	0.686864471
0.833025540	0.166585752	0.687122418
0.333221448	0.666672857	0.687177622
0.833174766	0.666634173	0.687249071
0.166301070	0.332952735	0.812445345
0.666188931	0.333142733	0.812867172
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0.331210720	0.166012750	0.981091524
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Interpolating coordinate: 0.833 (-823.188 eV)

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0.332264783	0.322405390	0.078789062
0.486468974	0.166798091	0.082668202
0.679189473	0.013757357	0.083293650
0.833260255	0.319947937	0.082854305
0.985381451	0.166289195	0.082492443
0.179473407	0.513643957	0.082672196
0.332816172	0.819721202	0.082682740
0.485599248	0.667456376	0.083164768
0.681098763	0.513592220	0.082842624
0.832638902	0.819550331	0.083029441
0.985814716	0.665931746	0.082765825
0.148732381	0.152748500	0.250022633
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0.349436821	-0.005428975	0.250935662
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0.846255638	0.000221081	0.249828637
0.153696435	0.652377411	0.249795625
0.000748821	0.847250436	0.249474787
0.346809232	0.499805131	0.249834458
0.656414767	0.657168498	0.250847817
0.501073805	0.845695553	0.249965167
0.848454969	0.501424184	0.250138951
0.013641510	0.180574007	0.417075506
0.320179423	0.333913296	0.416543629
0.166745163	0.486734903	0.416838934
0.514253103	0.180699657	0.417000870
0.820865111	0.334210026	0.417127565
0.668175331	0.487589924	0.418117206
0.014133574	0.680505873	0.416845752
0.319904388	0.832866132	0.417561843
0.167376342	0.986861408	0.416212997
0.514207408	0.680579355	0.417127439
0.821164642	0.834669197	0.417308587
0.666902912	0.986920168	0.417022297
0.486533306	0.319928784	0.583311531
0.180260834	0.166684787	0.583055938
0.333505482	0.013743269	0.583113324
0.986659862	0.319901305	0.583385538
0.680269606	0.166988520	0.583421203

0.833280471	0.013780380	0.583432639
0.486740184	0.819824978	0.583533121
0.180445014	0.666811044	0.583463863
0.333259408	0.513426029	0.583353717
0.987078771	0.820080726	0.583365441
0.680548412	0.667148351	0.583625751
0.833613358	0.513909272	0.583718794
0.346656710	0.346785607	0.749476829
0.152857041	-0.000190837	0.749414671
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0.152685182	0.499801713	0.749475728
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0.652789518	0.499903249	0.749829456
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0.318866894	0.487273481	0.914992367
0.165782967	0.180107588	0.915247436
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0.819229766	0.486238652	0.915984628
0.666506709	0.179942768	0.915951973
0.512891450	0.332486672	0.916167385
0.319036020	0.986260255	0.916032745
0.166290516	0.679770929	0.915879244
0.011666169	0.831532525	0.915008349
0.819113939	0.986104061	0.916289398
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0.001825007	0.000669758	0.145156635
0.497142098	0.000510510	0.146732697
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0.166605666	0.333394300	0.312055908

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0.000838375	0.000996894	0.352945619
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0.333781744	0.167219809	0.478432563
0.833357089	0.166923779	0.479112047
0.333866123	0.666453170	0.479216314
0.834535171	0.667882101	0.479365050
0.166731538	0.333338013	0.519995532
0.667057234	0.334041232	0.520378427
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0.666941714	0.833620231	0.520183444
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0.500032284	0.000058228	0.645853884
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0.833005290	0.166580331	0.687084721
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0.833140684	0.666642077	0.687220949
0.166306973	0.333030935	0.812364292
0.666040107	0.333049598	0.812811098
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Final coordinate: 1 (-823.203 eV)

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0.5140933706588912	0.3337346324280719	0.9156451349748240
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0.1667405782168549	0.6804750501115220	0.9161949033971186
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0.6665446685264939	0.6804540033705294	0.9166247826926250
0.5137120511917533	0.8338442770359172	0.9166109902777723
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0.8334269544105219	0.6668738230556800	0.6872846963461499
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0.3334537808214362	0.6672808151648340	0.9795782650318268
0.8332786451130790	0.6671672662016915	0.9797350256407779

(1.10) 2×2×1 supercell with the typical snapshots chosen from ab initio molecular dynamics simulations

Snapshot: 5 ps (-817.610 eV)

0.16501878	0.99554580	0.07420319
0.32462780	0.30615644	0.10108273
0.49114158	0.15662219	0.06885337
0.68336031	0.00605488	0.09128336
0.82746435	0.32017699	0.08771868
0.98993180	0.17099246	0.09120828
0.18920870	0.52086888	0.08261965
0.33650549	0.81396526	0.08567995
0.48681802	0.65208587	0.06659887
0.68607701	0.52017293	0.09121969
0.83871914	0.81777555	0.08508062
0.98761929	0.66681342	0.08805249
0.13511942	0.14464535	0.25292547
0.99614691	0.34310831	0.25560422
0.35146986	0.00228796	0.24191665
0.65389079	0.15294474	0.24980150

0.51431363	0.35568291	0.25031312
0.84257030	0.00358926	0.24842381
0.16637897	0.65866560	0.25977370
0.01318329	0.84837786	0.25254545
0.34779552	0.50078504	0.25012546
0.65627683	0.66230359	0.24840346
0.48881903	0.83864652	0.25525461
0.85637057	0.50710196	0.24642753
0.02067333	0.19287976	0.41803066
0.32780409	0.33089693	0.41480521
0.17253160	0.48435937	0.40999959
0.50781943	0.17379046	0.41814549
0.81311085	0.32841934	0.41631649
0.67043261	0.49042137	0.41572433
0.01808982	0.67380912	0.42430775
0.32535617	0.84270652	0.42102234
0.15615834	0.98096047	0.41778309
0.51857369	0.68787466	0.41136385
0.81981889	0.83870417	0.41527339
0.65625858	0.98351516	0.42024290
0.48031018	0.31553815	0.57633921
0.17641699	0.15968289	0.57934774
0.32919049	0.00401830	0.58835308
0.98341333	0.32231490	0.57392248
0.66414751	0.15932431	0.58013717
0.83647857	0.01573768	0.58431132
0.47080579	0.81394591	0.58522114
0.16801667	0.65699119	0.58490618
0.33315086	0.51081925	0.57618381
0.99675198	0.81692681	0.57979735
0.67168673	0.65817187	0.58169323
0.81969159	0.50717269	0.57679109
0.34013280	0.34289251	0.74833108
0.13959498	0.99473316	0.75437845
0.01242769	0.17001382	0.74818837
0.84594253	0.34406814	0.75521919
0.65700591	0.00061013	0.75470954
0.49643035	0.15184022	0.75579606
0.34978211	0.84307599	0.74863126
0.14544480	0.48307266	0.73486036
0.00794901	0.65761124	0.74238226
0.84443770	0.85861096	0.73843057
0.65334056	0.49570362	0.74335301
0.51458992	0.66376202	0.74338908

0.32201747	0.49412532	0.90877893
0.16278272	0.18331151	0.92523807
0.00753758	0.33766256	0.92459811
0.81415968	0.49693164	0.91142015
0.68064834	0.18510894	0.91749597
0.51769282	0.34863116	0.92225874
0.31528687	0.98237743	0.91844313
0.16961546	0.68410107	0.91353192
0.01029260	0.83258248	0.91206225
0.83534852	0.98625071	0.92323953
0.66611738	0.68021399	0.91057499
0.51720152	0.83866586	0.91019223
0.18252393	0.33180970	0.02327778
0.66144578	0.33638366	0.02271276
0.15575692	0.81647284	0.01868066
0.66928947	0.83101242	0.01843742
0.00442262	0.99502515	0.15048963
0.49847352	0.99887881	0.14856525
0.01188582	0.49640518	0.14392906
0.48956642	0.49690370	0.15188714
0.33841612	0.17379814	0.20528604
0.83681758	0.17079299	0.18798102
0.34173504	0.66907097	0.18880965
0.83264216	0.66991555	0.19187222
0.16532529	0.33305378	0.30968823
0.66148449	0.33295684	0.30715010
0.17459819	0.84004270	0.31025105
0.66816328	0.83539418	0.31639512
0.99694059	0.00561275	0.35474669
0.49422057	0.99883578	0.35206703
0.99769472	0.50579503	0.34764627
0.50437385	0.50603609	0.35348278
0.31834750	0.16598121	0.47148830
0.82565250	0.15681764	0.48139747
0.32981094	0.66568951	0.47921595
0.82729118	0.66393396	0.47943975
0.15695087	0.32943849	0.51550967
0.65593796	0.32550273	0.51731429
0.17360591	0.83481892	0.51981127
0.65844528	0.82140710	0.52281168
0.00921125	0.00000422	0.64271634
0.50218629	0.99757570	0.65177858
0.98958301	0.49103549	0.64156408
0.50112406	0.49541595	0.64312440

0.33738324	0.16703610	0.68449109
0.84336576	0.16974222	0.69178532
0.33081361	0.67011940	0.68213108
0.84875605	0.67556158	0.68303141
0.16377462	0.34244979	0.82026045
0.66441242	0.33237693	0.80681435
0.17794540	0.84231404	0.80923606
0.66746471	0.83399134	0.81126229
0.99943126	0.99629358	0.85635917
0.50412150	0.00363355	0.86775793
0.99640460	0.51071061	0.85447142
0.49620287	0.49864968	0.84536601
0.33160393	0.15549771	0.99262455
0.84015489	0.16485807	0.98250196
0.34655085	0.68565581	0.97652551
0.82194637	0.66621509	0.97726858

Snapshot: 9.5 ps (-818.601 eV)

0.18684197	0.02562763	0.08306683
0.33632205	0.33634652	0.08108277
0.47901388	0.17450809	0.08529500
0.68471386	0.00396830	0.09077348
0.81500768	0.31529652	0.08174240
0.98545148	0.16295147	0.07782186
0.17711570	0.50941351	0.08346864
0.32632664	0.81115730	0.07834537
0.48579555	0.66890089	0.08437604
0.68076785	0.51921502	0.08955995
0.84811920	0.82134206	0.08054064
0.98675255	0.66967485	0.08505246
0.15097896	0.16009482	0.24489038
0.98625590	0.33699185	0.24714731
0.35059752	0.01473477	0.25666863
0.64763045	0.14199148	0.24732620
0.49805774	0.35214578	0.25068486
0.84135098	0.98698518	0.24782427
0.15685943	0.65410155	0.24956705
0.99507438	0.84077808	0.24919196
0.33705660	0.49692913	0.25767205
0.65245297	0.64776153	0.25021209
0.48736011	0.84119969	0.25936488
0.85317194	0.49153503	0.24598442
0.01603422	0.17661415	0.41471219
0.31558171	0.32527626	0.41136958

0.15982125	0.48959829	0.41211859
0.51590520	0.18581709	0.41624983
0.81326678	0.32965989	0.42046738
0.66234399	0.49302218	0.41686587
0.01122771	0.67797793	0.42090166
0.32540128	0.84120111	0.42265120
0.16387298	0.98692836	0.41749935
0.51777758	0.68565480	0.41814542
0.81092292	0.83051531	0.41782803
0.67192861	0.99848520	0.41521465
0.48578149	0.31856722	0.58857329
0.19037594	0.16682972	0.58303920
0.33230723	0.00296793	0.59153853
0.98550310	0.31608786	0.57786414
0.67316393	0.16061992	0.58760384
0.82571380	0.01245494	0.58020534
0.48229056	0.81540348	0.59252409
0.18366133	0.66859914	0.58478841
0.34031940	0.50672940	0.57530675
0.98598890	0.82510806	0.58373395
0.67916753	0.67571252	0.58621219
0.82651043	0.51226197	0.58206579
0.35484074	0.34845336	0.76198136
0.15855140	0.99893368	0.75395187
0.00399363	0.15870459	0.74395842
0.84657263	0.35016194	0.74532602
0.65371605	0.99687292	0.74974283
0.49340926	0.16045827	0.75843754
0.35310232	0.84867764	0.74646597
0.15790467	0.50164620	0.74003870
0.00726101	0.65638643	0.74509389
0.85903712	0.85677803	0.75310248
0.65595894	0.50730328	0.75207127
0.50114169	0.65069622	0.75630624
0.30785653	0.49310283	0.92393919
0.16777020	0.17987109	0.91485137
0.00518599	0.32578559	0.90904823
0.82596333	0.47923207	0.91118153
0.66575742	0.17508563	0.91585337
0.50719150	0.32701107	0.91834546
0.31440227	0.98081677	0.91697772
0.15819862	0.67831593	0.91625544
0.99727857	0.83221452	0.91869333
0.83079571	0.00570712	0.90795621

0.67919420	0.68210534	0.91733317
0.51833757	0.83970672	0.91442545
0.17141446	0.33522507	0.02334377
0.65343532	0.32499146	0.01864895
0.17117452	0.84415052	0.02172999
0.67613126	0.83557776	0.02281877
0.99507752	0.99957425	0.13988576
0.50749086	0.00160568	0.13786772
0.99445060	0.48559108	0.14660942
0.51581276	0.51019264	0.14190109
0.33340658	0.17573470	0.18884886
0.82233286	0.15080905	0.18620359
0.33654862	0.66080189	0.19217785
0.83527950	0.65935891	0.19482868
0.15241137	0.32818720	0.31089794
0.66174362	0.33041976	0.30704239
0.17440685	0.83935255	0.31020759
0.66417169	0.83260977	0.30762509
0.99436617	0.99097809	0.35050618
0.49283339	0.99509484	0.35659484
0.98793550	0.49628082	0.35840561
0.49163613	0.49030716	0.35802272
0.33535256	0.16776547	0.48020870
0.83003065	0.16649595	0.47352013
0.32864800	0.66137095	0.48054840
0.82914399	0.67014788	0.47563851
0.16843530	0.33799169	0.51342820
0.65831609	0.32938538	0.51566289
0.16661557	0.82981835	0.52263080
0.65885760	0.83051900	0.51776606
0.00250719	0.01297411	0.64553669
0.50300962	0.00065279	0.65113033
0.98855531	0.49535928	0.64389963
0.49833598	0.49841438	0.64756928
0.33945330	0.16599121	0.69057148
0.83435090	0.17039410	0.68278918
0.34127373	0.67312748	0.69603652
0.83413426	0.66908857	0.68838352
0.17024692	0.32915709	0.81706144
0.66965772	0.33818680	0.81077573
0.16452226	0.83377129	0.81327812
0.68095040	0.84096996	0.81696169
0.00617286	0.00007757	0.85525231
0.50173841	0.00280881	0.85341641

0.01841324	0.50465331	0.84793181
0.50072026	0.50720895	0.86260959
0.33352789	0.16490292	0.97641567
0.83356285	0.17081773	0.97770142
0.34489575	0.68308506	0.98035113
0.84335288	0.65077238	0.98417499

Snapshot: 25 ps (-818.481 eV)

0.17090008	0.01414639	0.08594380
0.34756706	0.31879970	0.07679416
0.47110556	0.15761502	0.08718944
0.67207011	0.01292159	0.08378425
0.83381822	0.31658886	0.08131087
0.98829278	0.16218630	0.08285903
0.19171169	0.52536216	0.08457132
0.32078522	0.81599311	0.09164627
0.48583342	0.67777106	0.07709149
0.68684157	0.51067051	0.08911150
0.82978026	0.81910494	0.07801647
0.99489963	0.67582350	0.08917857
0.15130608	0.15088577	0.24984103
0.01897232	0.37255143	0.24960333
0.33557244	0.00102701	0.25802118
0.62967751	0.15501635	0.25088068
0.48876312	0.34449108	0.24680407
0.84007702	0.00127916	0.25102342
0.15253846	0.66282084	0.24993555
0.98921455	0.86071811	0.24827531
0.34797791	0.50181549	0.25028268
0.65095042	0.64641213	0.25179104
0.50273863	0.84505090	0.25126583
0.84216731	0.49730236	0.25145165
0.00897100	0.19006818	0.40756850
0.32524262	0.33861382	0.42358694
0.17784337	0.49771742	0.41472984
0.51849414	0.19263977	0.41252926
0.82060805	0.33398570	0.41057244
0.66569743	0.48449013	0.42695504
0.00850790	0.67171756	0.41734985
0.32385480	0.83798962	0.41875905
0.16230470	0.98640016	0.42346107
0.53428901	0.69226628	0.41237088
0.81973473	0.84204567	0.42290397
0.65889363	0.97706891	0.42015651

0.49067937	0.32713287	0.58557994
0.18839679	0.16602996	0.58326502
0.34084512	0.02084248	0.58235134
0.97987539	0.31705209	0.57678795
0.68310757	0.15944490	0.57536988
0.84321564	0.02339268	0.58597632
0.50511335	0.82723844	0.59078709
0.18944822	0.66494839	0.58714768
0.33436333	0.51344122	0.58661072
0.98840485	0.81594366	0.57920872
0.68633737	0.65925064	0.58429334
0.82416830	0.49706502	0.58839276
0.34558060	0.34618558	0.74891131
0.16606132	0.00089759	0.75016331
0.00922612	0.15347574	0.74531672
0.84616123	0.34273809	0.75097258
0.65472573	0.99708712	0.74557391
0.50230661	0.15389925	0.74706721
0.35210534	0.85455523	0.74373580
0.15673411	0.49678199	0.75280472
0.01126855	0.65037860	0.74095305
0.84248970	0.84568457	0.75308921
0.65387339	0.50451524	0.75699809
0.48915246	0.65416233	0.75234914
0.30631066	0.47435361	0.91884995
0.16996320	0.18209253	0.91980103
0.01055797	0.32549311	0.92075338
0.81333173	0.47760273	0.91520304
0.66374842	0.16871455	0.91832042
0.50655477	0.32495411	0.91208095
0.32054893	0.97859651	0.91563432
0.15973656	0.67664453	0.91999478
0.00871047	0.84146587	0.91783897
0.81063117	0.97981539	0.91387458
0.66268539	0.66490445	0.91261520
0.51877110	0.83144441	0.91320045
0.16426279	0.32429199	0.02365889
0.66327285	0.32796480	0.02360623
0.16960201	0.83948724	0.01916537
0.65948114	0.83097413	0.01869287
0.99109074	0.00183251	0.14653850
0.49435245	0.99152462	0.14463048
0.00280072	0.50337540	0.13964069
0.49937399	0.49896107	0.14943934

0.32230358	0.15515989	0.18422701
0.81999516	0.16320726	0.19418735
0.33040874	0.67330050	0.19400365
0.82817001	0.65697076	0.18975586
0.17395069	0.33850396	0.30954620
0.65466528	0.33928660	0.30548526
0.15980863	0.83965974	0.31708031
0.66486826	0.83571769	0.31117715
0.99417660	0.99200913	0.35250083
0.50275076	0.01356288	0.35465056
0.02048240	0.50970268	0.34785937
0.49868345	0.49800535	0.35288564
0.34293233	0.17814211	0.48306942
0.84012205	0.17312597	0.46917107
0.34773702	0.67345701	0.48261361
0.83447023	0.67039896	0.47729542
0.16407837	0.33720033	0.52131901
0.67357153	0.33588497	0.51419487
0.18372822	0.83699803	0.52233820
0.68080751	0.84471527	0.52983436
0.00568905	0.00230666	0.63928048
0.50882826	0.00530631	0.64313405
0.00052182	0.48893494	0.64146156
0.50489314	0.50912577	0.64887672
0.33634404	0.16765168	0.68696867
0.82298420	0.15721583	0.68497290
0.32624122	0.66681262	0.68713521
0.83974124	0.66218595	0.69673909
0.16570288	0.33127685	0.81208265
0.66677615	0.33130204	0.81069724
0.17087619	0.83655550	0.80994224
0.65901695	0.82776408	0.81254566
0.00005445	0.99832188	0.85390375
0.49587305	0.99858459	0.84968597
0.99524664	0.49220923	0.85899398
0.49291773	0.49697103	0.85769446
0.33120516	0.15436851	0.97703129
0.83107475	0.16381796	0.98407443
0.33043954	0.65784014	0.98067787
0.83447224	0.66369830	0.98008838

Snapshot: 37.5 ps (-818.210 eV)

0.19193802	0.01924579	0.08049646
0.32645358	0.31254775	0.08250722

0.48203952	0.16246722	0.08331357
0.67998819	0.01941001	0.07742860
0.83135910	0.31972121	0.08875437
0.97597081	0.16984450	0.08189932
0.16768435	0.51305323	0.08408478
0.33389512	0.81566735	0.08489118
0.47961871	0.66639936	0.08701565
0.67406095	0.50972461	0.07542997
0.83577435	0.82359135	0.08035529
0.98493438	0.66894606	0.08214320
0.16839084	0.17770227	0.24802023
0.99458881	0.34178403	0.25169374
0.34744412	0.99720380	0.25028888
0.64786889	0.14841623	0.25407214
0.50673174	0.34209577	0.25152875
0.83449062	0.99269899	0.24481076
0.14408093	0.65284723	0.25226292
0.00724773	0.85172926	0.25191655
0.34671855	0.49910010	0.25248096
0.65074106	0.64884806	0.25039464
0.50652878	0.84449376	0.23423627
0.85523385	0.50473640	0.24865657
0.01394547	0.17816073	0.41197313
0.31988758	0.32828820	0.41564378
0.17188649	0.47987065	0.42098793
0.51205427	0.17942303	0.41865732
0.83152643	0.33324071	0.41783250
0.65539294	0.48691414	0.40840506
0.00758801	0.67666599	0.42612446
0.32884488	0.83664376	0.41466664
0.16491472	0.98778288	0.41408233
0.51100012	0.68388401	0.41266895
0.82089961	0.84040963	0.40848901
0.67403284	0.98440929	0.42162974
0.47729570	0.31155265	0.57802518
0.18241435	0.15266052	0.58237863
0.33937350	0.00219965	0.58427085
0.97916345	0.30690037	0.58505948
0.68494960	0.15838008	0.58228744
0.81705858	0.00085236	0.58827404
0.48655698	0.81972890	0.58495528
0.18381779	0.66283650	0.57949542
0.32512026	0.50417042	0.59032701
0.97893410	0.81321826	0.58381946

0.68028497	0.65960211	0.57415552
0.83775735	0.50787549	0.57506078
0.34438577	0.34191569	0.76040807
0.14390445	0.99281638	0.75226130
0.00330788	0.15953084	0.75009425
0.85095853	0.34985754	0.74203775
0.65995154	0.01066800	0.75564864
0.48918933	0.15820352	0.75303592
0.36443525	0.84791243	0.75768304
0.14542151	0.50239056	0.74890539
0.01373458	0.66629562	0.75150795
0.85388487	0.85228208	0.75363534
0.65062905	0.50123613	0.75295500
0.49857359	0.64953862	0.75071622
0.31736825	0.49603671	0.91854730
0.16653835	0.18780341	0.92723394
0.00597791	0.32638257	0.91631957
0.81722393	0.48332412	0.91048388
0.66708088	0.19244196	0.91770586
0.51647603	0.33920947	0.91913804
0.32416644	0.99834041	0.90658325
0.15718370	0.68164721	0.92151002
0.01388816	0.83751236	0.91718363
0.80715592	0.97815141	0.91277408
0.66002099	0.68084373	0.91751305
0.52057164	0.84399061	0.91656770
0.16182516	0.33834507	0.02556674
0.66429706	0.32921934	0.03029565
0.16641461	0.82899800	0.01802400
0.66624464	0.82886234	0.02991390
0.01273744	0.00748094	0.14680382
0.50739780	0.00130189	0.14835787
0.98952214	0.49686111	0.14945671
0.49937372	0.49286306	0.14601124
0.33663333	0.17539711	0.18091576
0.83979464	0.16999023	0.18690439
0.32630881	0.65723751	0.17918449
0.84444063	0.68942157	0.18446607
0.16701062	0.33855958	0.31284747
0.67765494	0.33852540	0.30967679
0.17450074	0.83890448	0.30785866
0.66769749	0.83731739	0.30322269
0.99745372	0.99578208	0.35218652
0.51743667	0.00927592	0.36730811

0.01156592	0.51098049	0.35855429
0.49786138	0.50220995	0.34977951
0.32882887	0.16259290	0.47720629
0.84543341	0.16566915	0.48278711
0.33815383	0.67701639	0.47222080
0.82407853	0.66571186	0.46961626
0.16466434	0.32136692	0.52483330
0.66708599	0.32304786	0.52156411
0.15874815	0.83049642	0.52623766
0.67231463	0.83174435	0.51580003
0.98617664	0.98874198	0.65263410
0.50204272	0.99538852	0.64811202
0.00931864	0.50484762	0.64105648
0.48889538	0.48314595	0.64303768
0.32271011	0.15818980	0.69180940
0.83598772	0.17090847	0.69065145
0.33998846	0.66976197	0.68778537
0.83289662	0.66099785	0.67943295
0.16207179	0.32732330	0.81621175
0.65904259	0.33306100	0.80729762
0.17622234	0.84259765	0.81520070
0.65746385	0.83499400	0.81149011
0.99516904	0.99788632	0.85938261
0.50418579	0.00484509	0.85638606
0.99563853	0.50911334	0.85166563
0.50514839	0.49585556	0.85620136
0.32930029	0.16343685	0.97648949
0.82874563	0.16607512	0.98239958
0.33349991	0.67114370	0.98127828
0.82595573	0.66171946	0.97733797

Snapshot: 40 ps (-818.801 eV)

0.16256460	0.99548428	0.08035444
0.34585574	0.31542915	0.08532152
0.49498229	0.15836491	0.07179434
0.68330176	0.00883887	0.09413540
0.84891497	0.32007437	0.07501609
0.98626633	0.15974458	0.08937946
0.18549801	0.51021717	0.09264822
0.34588412	0.82528301	0.07596921
0.49583083	0.66995100	0.07720177
0.67817741	0.50591263	0.08402754
0.84261577	0.82544503	0.07721141
0.98768026	0.65929195	0.08019372

0.15046452	0.15490546	0.25397021
0.00036028	0.35042393	0.25377657
0.33942651	0.99138106	0.24911882
0.65510112	0.15923834	0.25846057
0.50701469	0.36059810	0.25224073
0.84000380	0.99617631	0.25274611
0.16042908	0.66212065	0.24546328
0.00185351	0.85381036	0.25186438
0.35356756	0.50307444	0.25101348
0.66026972	0.66408901	0.25330145
0.49824485	0.84764375	0.25604623
0.84921513	0.50531677	0.24690109
0.02129507	0.19519494	0.41253257
0.32766447	0.33767100	0.41741736
0.16874589	0.48847596	0.41693639
0.51111429	0.18866917	0.41442720
0.81310072	0.33787447	0.41152989
0.66284444	0.48771123	0.41679738
0.00123602	0.66242041	0.41647038
0.31957433	0.84091483	0.42327937
0.15768092	0.98117173	0.42562059
0.51183325	0.68826070	0.42771050
0.81790780	0.84172812	0.41591122
0.65837675	0.98843010	0.41847464
0.48870554	0.31889511	0.58139564
0.16595269	0.16841997	0.58127046
0.34116095	0.01375717	0.58198193
0.98592322	0.32113992	0.58794616
0.67817566	0.16859098	0.57860943
0.82401022	0.01878281	0.58097893
0.48756541	0.82104366	0.58907768
0.17297679	0.66056256	0.57830687
0.33120899	0.50333377	0.58707468
0.98733255	0.82666278	0.57967949
0.68276113	0.67353784	0.58739255
0.83102363	0.52119166	0.58712688
0.34757491	0.34605549	0.74994899
0.14689617	0.99657398	0.74427024
0.99267579	0.13976324	0.75103941
0.85266294	0.35223304	0.74301045
0.65464129	0.00102068	0.74665736
0.48945017	0.14917365	0.74454703
0.34543248	0.83670147	0.75510413
0.16276149	0.49785315	0.73898122

0.00152226	0.64748816	0.74851637
0.85028886	0.84121783	0.75493771
0.64397997	0.48214249	0.74985578
0.51002586	0.65298190	0.75348615
0.32323911	0.49280731	0.91182482
0.15729077	0.17246312	0.91563754
0.02216716	0.33949942	0.92420892
0.81780130	0.48751019	0.91521890
0.66814838	0.16427128	0.90459655
0.50449614	0.32787744	0.92022234
0.32063363	0.97859182	0.91808765
0.17635483	0.68820022	0.91214857
0.02317248	0.83859152	0.91766579
0.82096336	0.99648230	0.91756156
0.66952305	0.67870506	0.91515868
0.53641808	0.84643455	0.91343763
0.16943049	0.32758889	0.02966924
0.66978176	0.33347665	0.01725745
0.16133604	0.82052649	0.01620338
0.67394617	0.84484386	0.02158500
0.01002786	0.00930117	0.15513622
0.50491319	0.01096246	0.14724122
0.00620535	0.49596043	0.14883016
0.50626303	0.49866732	0.15063802
0.33289992	0.15951784	0.18801603
0.83602473	0.16510534	0.18656305
0.34864177	0.67320023	0.18674968
0.83573417	0.67252162	0.18740459
0.17621473	0.33366256	0.31358436
0.66274428	0.34191451	0.30537537
0.15558762	0.82710321	0.31187778
0.66471862	0.83778391	0.32587226
0.99697085	0.00352157	0.35431967
0.49062781	0.99930385	0.35268690
0.00768625	0.50239962	0.35199463
0.49640795	0.50904629	0.35781287
0.33105772	0.16759835	0.47760824
0.82289786	0.16976442	0.47285582
0.32967911	0.67592200	0.48688927
0.83387053	0.66503356	0.47800169
0.16100536	0.33705118	0.51870801
0.67159856	0.33845419	0.51418911
0.16308061	0.84145843	0.52541000
0.66407879	0.83440456	0.52417813

0.98476720	0.99187680	0.64816888
0.51163219	0.01124098	0.64334547
0.99328310	0.50477112	0.63998834
0.50003993	0.49576783	0.64449597
0.32310118	0.16231888	0.68593455
0.83873776	0.16728440	0.68436264
0.33915709	0.66723003	0.68601555
0.82263037	0.65244266	0.69405622
0.16856513	0.33147995	0.81100235
0.66297922	0.32115680	0.81165291
0.16535793	0.83261686	0.81076532
0.67068967	0.83064777	0.80915780
0.99773188	0.99841418	0.85668114
0.50192312	0.98812211	0.85254091
0.99339447	0.48933681	0.85534549
0.50038830	0.50050664	0.85193605
0.31927744	0.14505387	0.98093867
0.83702893	0.16817133	0.97429733
0.34121038	0.66897944	0.97816365
0.82929814	0.67149507	0.97685701

(2) Si@EP-Fe₂O₃

(2.1) 2×2×1 supercell with the EP localized on Fe1 (-829.858 eV)

10.1413002014000000	0.0000000000000000	0.0000000000000000
-5.0706501007000000	8.7826236017999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.9027004242000007

O	Fe	Si
72	47	1
0.1852597094262997	0.0163100845483613	0.0850694260350203
0.3324235780448301	0.3197457251547390	0.0842269381227621
0.4874127121802198	0.1674006641282402	0.0844637035981047
0.6804381314677047	0.0129713147209025	0.0843166417247695
0.8345126560043925	0.3222669409531168	0.0858925866834335
0.9842134267051003	0.1742717440001440	0.0824769107959521
0.1796393556952068	0.5146913700196987	0.0839090020926492
0.3335623519170481	0.8194440412252807	0.0844222164454812
0.4830621704847896	0.6627739334316222	0.0857586609344587
0.6788741452968879	0.5090208928575554	0.0830729876144729
0.8221001582668690	0.8065231084279444	0.0820357530872148
0.9870668214175093	0.6690029137840428	0.0834114314414733
0.1609262305293208	0.1780515570189322	0.2606859907112975
0.0172803931496926	0.3431062874581790	0.2589295622242428
0.3470689353999330	0.0024447267617426	0.2512297207044198
0.6561877735764262	0.1530950670743975	0.2503867406229499

0.5007622968178487	0.3479052769934449	0.2496203220828493
0.8465231473835113	-0.0015239896155017	0.2499705064626469
0.1521183261370685	0.6526721878486135	0.2498585425885110
0.0001473718543373	0.8445292946871839	0.2541458585068425
0.3264848284295498	0.4845351301665262	0.2589878380040375
0.6477726909342889	0.6501333913881768	0.2497191511584183
0.4975598325693182	0.8444923776873520	0.2509179481394150
0.8497001753467341	0.4981824676421842	0.2491123329445500
0.0229769852850704	0.1912021667818427	0.4104499111519438
0.3106115204699557	0.3335229685481999	0.4115526385300805
0.1686123056436227	0.4778058468589493	0.4102138249087040
0.5127489303613528	0.1809130445051836	0.4159534028532043
0.8197227122503857	0.3337798406960159	0.4160998520593993
0.6662982075002024	0.4866577633083360	0.4159089237664717
0.0143628529405047	0.6780928455171391	0.4176831558751842
0.3202867705086996	0.8323483922274439	0.4165874367539736
0.1663146159325015	0.9860454580958760	0.4166863011428058
0.5144753871840074	0.6803435112186679	0.4166094471610683
0.8210187325052316	0.8352055986330826	0.4163099129971857
0.6678379171466110	0.9877155640262324	0.4164110521394014
0.4843057362555999	0.3201831636418789	0.5810728524645407
0.1796383710354916	0.1658656799809513	0.5825982408057737
0.3335249313013355	0.0138929077571194	0.5824169314537059
0.9863371479897197	0.3205238096252156	0.5822433446127732
0.6804645062232941	0.1668001130365180	0.5821858596420810
0.8361599893337908	0.0161252202194075	0.5812929458364964
0.4865863140719502	0.8197922337701096	0.5823418992320442
0.1801601593604236	0.6641084119562678	0.5813533889796640
0.3340753516381485	0.5137915085522401	0.5824425355480087
0.9866791644459112	0.8194211974354337	0.5831929318754069
0.6808184859180041	0.6674093912031164	0.5828812867245550
0.8325004186712093	0.5132675650452145	0.5830156224180287
0.3463042674428694	0.3466687723687629	0.7493288017791985
0.1533001220614189	0.0002227405122298	0.7498154513307782
-0.0001002203459345	0.1531533621953271	0.7495679646909822
0.8466775244241891	0.3468348939769526	0.7493719140091248
0.6531349111005702	-0.0003653092403689	0.7493470966576714
0.5003661321747044	0.1532957151415706	0.7491901638635408
0.3466532805426753	0.8470143721539104	0.7492267210280978
0.1530401762720148	0.5000054252570589	0.7492207964649508
0.0004467124429329	0.6535285143017134	0.7494572718915730
0.8467685137661798	0.8470559565238852	0.7495751757425139
0.6526129260627510	0.4993036588309076	0.7492265763397737
0.4997363231869868	0.6530291423617062	0.7492484288531971

0.3193783526806735	0.4867939392985325	0.9166424290780412
0.1664165462536026	0.1804177908152376	0.9171755170391884
0.0135523465397541	0.3340360697784153	0.9158007139495529
0.8197620556611859	0.4859940904832837	0.9164262576578807
0.6667648482262133	0.1797968604171060	0.9169816143611147
0.5130708201677685	0.3327463003166740	0.9163924694466520
0.3202308102648387	0.9867444705718618	0.9167312927212005
0.1666640423395184	0.6806551035914404	0.9166855770756800
0.0136974091667441	0.8338669250069451	0.9170338095662424
0.8191779810320085	0.9852943060375445	0.9170153669320157
0.6646096875862112	0.6788213749951221	0.9154534797707913
0.5126038460207729	0.8327299635661626	0.9169397631231042
0.1652372378865681	0.3335203558346036	0.0213867137627135
0.6673991382143475	0.3312079258371842	0.0210428259311438
0.1685924131063290	0.8362895819113599	0.0215161630928898
0.6641737236351090	0.8312800310310997	0.0217274886657116
-0.0020049914341373	-0.0034376730164282	0.1432827346604270
0.5010112344057719	0.0009661955421873	0.1464513967574395
0.0005692853985496	0.5044968731080589	0.1445333773207509
0.5028887244201257	0.4971756123975759	0.1441681834095554
0.3290551742898880	0.1681282200200310	0.1894116401768411
0.8410716208176284	0.1682949802914738	0.1881724594336167
0.3307185238996527	0.6619982358434982	0.1889796916852459
0.8354328381919540	0.6725974292558811	0.1870274554891828
0.6671723529861532	0.3328509959378916	0.3113034006670586
0.1677803374496027	0.8332960263389807	0.3134409608884815
0.6666966898258446	0.8341171543477491	0.3124870697813440
0.0015420830675765	0.0009051121981949	0.3498943992124922
0.5004312900593437	0.0005508805605507	0.3534577940519070
-0.0003456663846943	0.4993295264213302	0.3523481403858594
0.5000850314464163	0.5004012481472699	0.3526509168426095
0.3316567876054387	0.1655192347468392	0.4781617574377575
0.8343585179054288	0.1685093077861091	0.4779872815521404
0.3350351605136452	0.6664135540715381	0.4784283916195142
0.8337860737979098	0.6673274504270462	0.4786498759296215
0.1667788219417419	0.3331480513392982	0.5237098024303231
0.6659016440231965	0.3336717113049547	0.5199221531026779
0.1665452960704009	0.832323218435297	0.5205652055403264
0.6682837613987619	0.8345977070237646	0.5201626448390084
-0.0002562031504752	-0.0007557438541711	0.6464132840078681
0.5002196740676007	0.0001322283835436	0.6456083983514427
-0.0006450950374784	0.5002182613243188	0.6460147814989758
0.5008392950272436	0.5006156348444358	0.6459687475219964
0.3334473407703586	0.1666238346382275	0.6871309050945629

0.8331596386133476	0.1666156444199299	0.6870612005921588
0.3332904241981375	0.6668271613070692	0.6870415703713827
0.8331737964518510	0.6665477804015076	0.6871722212084670
0.1661996997978152	0.3334351474792982	0.8131082374223362
0.6666790346455906	0.3333341035754428	0.8131097356115672
0.1667947695619371	0.8336275637885986	0.8131534538762819
0.6663246095516279	0.8326880561651469	0.8130817023394734
-0.0000138002985834	0.0003051233616631	0.8547469773156974
0.5003804878043511	0.0000308672801681	0.8541879511380644
0.0000698952226920	0.5004675326937548	0.8539227211916349
0.4984486293474411	0.4986376677811525	0.8537989721317238
0.3336192221166527	0.1669933269960238	0.9805582029094255
0.8346024125185235	0.1663515414030890	0.9802197888600864
0.3323698045148429	0.6665263004212161	0.9800257412582107
0.8313658329457239	0.6662378518085499	0.9788651543396157
0.1675931087137136	0.3345558339641834	0.3211092952610840

(2.2) 2×2×1 supercell with the EP localized on Fe2 (-829.732 eV)

0.1788926717372877	0.0148370954621372	0.0857429448344644
0.3320759315534861	0.3217893941193545	0.0837728172104332
0.4834178944338581	0.1745288349180456	0.0830920560171833
0.6868437111641242	0.0146846038949891	0.0843051451789530
0.8351088449212078	0.3205335258297259	0.0860962889076006
0.9878437123035072	0.1671170147647315	0.0838144295736363
0.1775745839285222	0.5098452028086258	0.0835352211598035
0.3230552192311932	0.8081022181513182	0.0827402112023860
0.4849653585537412	0.6648036584233866	0.0860146570353275
0.6810332535902933	0.5146099786279454	0.0835029390406491
0.8326877915413283	0.8188086590246095	0.0835228146275099
0.9849239389270704	0.6669005108633981	0.0832178157285073
0.1576539106581026	0.1738577032325955	0.2578464237026534
0.0172571565663180	0.3429684691320785	0.2581710766059687
0.3460806036412928	0.0021031386626194	0.2511348042087593
0.6620323334929644	0.1579319793586105	0.2544767844795756
0.5016192338251034	0.3487803096383202	0.2499719244068078
0.8475338602923139	-0.0013638221460999	0.2500528035227539
0.1511282415100708	0.6528052758227725	0.2498321398169942
0.0017807932319621	0.8511449204995560	0.2496419646875552
0.3263356005116878	0.4831676248263336	0.2578863400042570
0.6492861867578305	0.6502370900424401	0.2498875081429141
0.4965558251136197	0.8386274411173944	0.2549706119724734
0.8500775500127710	0.4991430995308506	0.2497492170828889
0.0226512019672980	0.1912073559658038	0.4097877602463676
0.3089680602711902	0.3311875665481946	0.4097935225622190

0.1691715258966572	0.4778715431442008	0.4098011248016355
0.5129297038411804	0.1804775677419652	0.4161512927929983
0.8214842945813194	0.3358596271789333	0.4177399778727053
0.6656390559691115	0.4865913235771747	0.4166144940405498
0.0138826402859314	0.6793904334380950	0.4164543542728754
0.3198020926126961	0.8328107376148346	0.4162256669333306
0.1657787746629734	0.9859969239767898	0.4166425476790834
0.5147190274880400	0.6788545336847158	0.4178634218155298
0.8214894280933975	0.8346235688135372	0.4166243679574108
0.6682508588060742	0.9871360595148283	0.4167401519172349
0.4840915187595480	0.3201117139215355	0.5810857903657398
0.1796687662804474	0.1660658487333596	0.5821752782349018
0.3333944843039959	0.0138344142569924	0.5825143961551070
0.9866071063383337	0.3203695927144445	0.5823219461049358
0.6804039327187403	0.1666361389709249	0.5825749656387477
0.8361678345407703	0.0160467384865081	0.5812783369751613
0.4862112961115926	0.8196570302682403	0.5825779570173504
0.1799637083875602	0.6639894142228991	0.5810127766961835
0.3339080018163475	0.5135468643231367	0.5823142470780889
0.9869209149943838	0.8194594730974503	0.5831125329311863
0.6809077074713125	0.6675133983573195	0.5833584232425340
0.8325866591377539	0.5133992121669082	0.5832264266107313
0.3466320554871739	0.3469930024890228	0.7491871873124115
0.1533364637716872	0.0000586353451849	0.7495925772587387
0.0001419232903556	0.1532145946983825	0.7493061158275648
0.8463682054607820	0.3465112738211230	0.7495765360250232
0.6530601830832019	-0.0000946755711418	0.7496382299402624
0.5001021003012074	0.1532429295894600	0.7495638236805463
0.3467295820322129	0.8468974630820624	0.7494628809626622
0.1528982968192632	0.4996178769463638	0.7491237356308917
0.0001371389771356	0.6530567573765035	0.7491578580741405
0.8467555703737755	0.8472278704346233	0.7494641389802174
0.6527579732742496	0.4997966243887136	0.7493592249463805
0.4999661534303764	0.6535212388041460	0.7496245420356501
0.3192486114344260	0.4865614301466094	0.9164031651183936
0.1667935018195739	0.1803335075357039	0.9164905862099226
0.0125964990129143	0.3324876207572348	0.9164209482603388
0.8197712807511836	0.4863190608223523	0.9165857800658522
0.6662983337928250	0.1800695894311941	0.9177782859113042
0.5141348155182125	0.3345348789430064	0.9157851756576131
0.3195320009662316	0.9863644569039426	0.9173203338017616
0.1650865480329478	0.6796005998028152	0.9154228150000649
0.0131217858261882	0.8335283732315690	0.9164563183140778
0.8196946397267444	0.9859417388654820	0.9164052467831594

0.6660727414236260	0.6800613501146763	0.9167065364939855
0.5130899959483591	0.8331874805294551	0.9176399597324527
0.1661765672822054	0.3328624725150636	0.0203969963233560
0.6661230104699066	0.3318493945428025	0.0221462234399285
0.1673400499288414	0.8350311533328211	0.0213690857431923
0.6647153296804810	0.8327706769834174	0.0217657565032391
-0.0031634863315703	-0.0005747275811494	0.1447821925215936
0.5006028479957957	-0.0032927458777608	0.1447831363088128
0.0027156143790963	0.5036529926390310	0.1444236305801180
0.5001196608175861	0.4976285028040590	0.1449612835666341
0.3350593985367520	0.1687688794415966	0.1876709437496091
0.8356976574021372	0.1674779891590918	0.1894983660477022
0.3323104086533227	0.6671242582484044	0.1881347739363384
0.8333290059641375	0.6666876023064161	0.1875539977870380
0.6673612801967959	0.3334504309270859	0.3130791216374255
0.1681932734838991	0.8345785214745485	0.3125793909720576
0.6665841146223994	0.8328293259434094	0.3134418380799234
0.0009057904647529	0.0010128474705202	0.3525000634211795
0.5015621875496455	0.0004043298307488	0.3504997264381408
0.0007785810563211	0.4999029523386608	0.3526742990129859
0.4991741716302473	0.4996585233338646	0.3526551984048409
0.3321671026443699	0.1652365696469876	0.4779755999352328
0.8337938603923147	0.1684781519460142	0.4781121077286168
0.3350218394316053	0.6668949583456908	0.4778644845521723
0.8335681301749065	0.6667284891850420	0.4791613556373923
0.1668303810060022	0.3334203900391061	0.5230156223362069
0.6658496813935842	0.3334038264066773	0.5203348606798641
0.1668051172426117	0.8323896223417723	0.5201468408845320
0.6677757796853226	0.8343704771617453	0.5205956925978720
0.0000192614456832	-0.0006153233789364	0.6460626446387868
0.4999672126941179	0.0000450669226932	0.6459376985830216
-0.0005519325254839	0.5001592184559278	0.6459454121466707
0.5006751329044399	0.5005519186130702	0.6459935392510734
0.3333701223176695	0.1666849723084743	0.6870523032480993
0.8332324196426731	0.1665772416050725	0.6871139948322782
0.3332532052001453	0.6666597782405198	0.6870067904448964
0.8332320452183801	0.6667358872760799	0.6871800081230995
0.1665371912522023	0.3332973085449512	0.8129020950127399
0.6662970726890565	0.3335473938693505	0.8132340206480051
0.1663197651118437	0.8328679727875237	0.8129279370349823
0.6668766204744095	0.8336112579205978	0.8132284911223842
0.0004271759866163	0.0005547131493686	0.8540493944605820
0.4997896137269438	-0.0000749355265223	0.8549739687300602
-0.0007614101764191	0.4988865415169609	0.8537578363074518

0.4992820091972399	0.5003750270136949	0.8538679779344212
0.3352721825941553	0.1685377967744310	0.9800108309572361
0.8329494605855727	0.1651894918421530	0.9806319396100515
0.3303494759924157	0.6661885901577856	0.9800558086271531
0.8329881972435114	0.6664094812559148	0.9785222277022496
0.1673884462804165	0.3334298779322323	0.3191278826427081

(2.3) 2×2×1 supercell with the EP localized on Fe3 (-829.858 eV)

0.1797114201418048	0.0169367750822984	0.0857589161566067
0.3350524116185986	0.3203603419254974	0.0839087471534259
0.4858816850719436	0.1664372007170923	0.0844219171674507
0.6799877402670635	0.0125870347423779	0.0844631249480857
0.8310519672437329	0.3147406153512771	0.0850684492691136
0.9873221890468821	0.1675753163701961	0.0842265503299077
0.1900570968992147	0.5157844510900138	0.0824772203041582
0.3325330847491346	0.8195607633168035	0.0843169726635443
0.4877536734494661	0.6654866733000966	0.0858927738375791
0.6819361949926628	0.5129320538887988	0.0834118201256455
0.8301459568303537	0.8211251762093149	0.0830731222575563
0.9844221777494027	0.6778993441464882	0.0820366696399052
0.1580513179646742	0.1735167012767987	0.2589885285618598
0.0171260742989335	0.3390754950316580	0.2606863954738678
0.3469333950344967	0.0024411156776071	0.2509181186004612
0.6553769187133982	0.1529324418079856	0.2512292873267570
0.5005541633953137	0.3478821205593177	0.2498580398407043
0.8471431353725825	-0.0007612608711892	0.2496195898664748
0.1519532812223580	0.6534779989956296	0.2499705971239222
0.0023611785599317	0.8522276859708441	0.2497197417162747
0.3258265366459121	0.4827204274721549	0.2589298197134689
0.6484830274945075	0.6503010155737876	0.2491128146691977
0.4969071687335386	0.8438131328650561	0.2503866296886267
0.8443826629773610	0.4998537610002534	0.2541464200676281
0.0229123757731902	0.1893904320436996	0.4115523581448192
0.3091944460941363	0.3313895499481192	0.4102137311945959
0.1682261684910377	0.4770244938451262	0.4104499923690233
0.5120628427880145	0.1797151915227078	0.4165869767121370
0.8197315284643313	0.3336867611261847	0.4166864859615643
0.6637300536599352	0.4856386697414132	0.4176833359942997
0.014188022206568	0.6789823895511957	0.4163105607653688
0.3198782824744149	0.8321637326226776	0.4164106439304860
0.1658682514375866	0.9855256600137658	0.4166097404604641
0.5140580803896775	0.6802794611695793	0.4160996587545474
0.8203608186647182	0.8337037470634296	0.4159088078115723
0.6681648246734087	0.9872521810588881	0.4159526285011583

0.4839479899126401	0.3198402722220306	0.5813528141609429
0.1797158897027689	0.1659254205122833	0.5824424272820825
0.3332068335370112	0.0134153358961893	0.5823419882410823
0.9862282354353769	0.3203629355456512	0.5825975872035719
0.6803676797859760	0.1664754455713998	0.5824169364983525
0.8358778771909273	0.0156954688418700	0.5810724938458894
0.4863357387622702	0.8195363284165224	0.5821860792332092
0.1799659009877799	0.6638409185699770	0.5812928932300422
0.3341874487903508	0.5136641149748857	0.5822429342896854
0.9865909311977635	0.8191821679075859	0.5828817219681041
0.6807676875448450	0.6675009408504484	0.5830160355884112
0.8327428569388658	0.5133221644768641	0.5831927513416989
0.3469638996665117	0.3469583333368738	0.7492202562356014
0.1532922620085580	0.0002622137296621	0.7492488170573202
0.0003635272991737	0.1536947622328406	0.7493286459968317
0.8469213190459245	0.3466989848293553	0.7498151039760396
0.6529283336416715	-0.0003681284244746	0.7491903987311948
0.5003606119400498	0.1533453019726448	0.7492266543592955
0.3464988813313779	0.8468641455399638	0.7493477868969620
0.1532530215420571	0.5000984762452445	0.7495676080272219
0.0002871120954875	0.6532302164638230	0.7495754316965937
0.8466902207417345	0.8473861912497679	0.7492268529198033
0.6530807637910921	0.4995519442831537	0.7494569046603181
0.5001567061898581	0.6533211108697604	0.7493722826743922
0.3204833915043675	0.4864465303987460	0.9158007446485893
0.1674145680739071	0.1806197793373082	0.9166420707061546
0.0140005661839509	0.3335821220034001	0.9171748542629437
0.8201682279932014	0.4863012479072982	0.9170337700580241
0.6665128258552608	0.1797679262175901	0.9167305771313051
0.5139897900979620	0.3333337469782661	0.9166851398290052
0.3201251158832294	0.9873935137202129	0.9169400693074055
0.1661151136888439	0.6808198029507537	0.9170161272925336
0.0142109036283130	0.8353882025108983	0.9154540373125111
0.8196746635998078	0.9869280754292928	0.9163923547581740
0.6662309371194206	0.6802362288659493	0.9164267871340086
0.5130313981882019	0.8332338527103151	0.9169817305497023
0.1682832813816666	0.3347613315030038	0.0213867825940289
0.6676979052682455	0.3314065687330132	0.0215157668129035
0.1671055276017891	0.8358254282285241	0.0217279656821874
0.6638074133626551	0.8326002749222692	0.0210425287312035
-0.0057141949859939	-0.0028900995008015	0.1441679728607390
0.4999545580281067	-0.0010114722604523	0.1464516718931843
-0.0014321117926131	0.5020064967478577	0.1432839561874951
0.5039288165770462	0.4994307528483520	0.1445331754508949

0.3312793974558942	0.1692822099278291	0.1889797738158374
0.8390742853370960	0.1709470239195933	0.1894113289797764
0.3272239910012557	0.6589280294392590	0.1881724451819399
0.8371643975939732	0.6645676977649496	0.1870274915392331
0.6655161176713184	0.3322206080431900	0.3134405752482013
0.1674209382966503	0.8333042929738008	0.3124868971687123
0.6656795683815130	0.8328293361324087	0.3113025093756152
0.0003176793912297	-0.0000835802969108	0.3526505341770962
0.5001199278423780	-0.0004305509816575	0.3534575827852995
-0.0006364213615746	0.4984590311736902	0.3498952951303492
0.4996763656107893	0.5003477274009061	0.3523478158550233
0.3313783797453490	0.1649652075338358	0.4784285561649447
0.8338630667458463	0.1683447744218362	0.4781616886000132
0.3341521815414623	0.6656427850591397	0.4779872250856134
0.8335418333297399	0.6662151900794190	0.4786499430336319
0.1663705969685633	0.3332223784234333	0.5237102927001456
0.6657779448159706	0.3334559919206221	0.5205652123484874
0.1663148411070198	0.8317173002615733	0.5201625402726612
0.6677704383795884	0.8340988666602664	0.5199216061508557
-0.0002236049183810	-0.0008394166304860	0.6459686898477843
0.4999122370955247	-0.0002196098201009	0.6456088329258145
-0.0004995025769197	0.5002568999708273	0.6464133514442192
0.5008640057910998	0.5006454227022237	0.6460145664541276
0.3335358250818015	0.1667082364309717	0.6870414177025740
0.8331753586457906	0.1665519606513035	0.6871309290822063
0.3334559104742611	0.6668405608322233	0.6870614556244345
0.8333734800172453	0.6668255180229572	0.6871726328648782
0.1672351348895870	0.3337993788104895	0.8131084452208636
0.6668313310105983	0.3332042424469110	0.8131527900408990
0.1663623503379601	0.8336739889803153	0.8130822715087573
0.6666546186107392	0.8333199303697318	0.8131096003249667
0.0001882767392160	0.0015499191198423	0.8537988785660399
0.4996497186706393	-0.0003815467287974	0.8541873112504281
0.0003175795492908	0.5000118656538591	0.8547469517670264
0.5003972196528547	0.4999286826596521	0.8539225699588910
0.3341567343116136	0.1676291323656181	0.9800260399148785
0.8333742732378226	0.1663794837519554	0.9805581452659063
0.3317477356281003	0.6653952078975212	0.9802200231018189
0.8348708168670133	0.6686328870432408	0.9788653527233586
0.1669642210882931	0.3324087340395124	0.3211098473768218

(2.4) 2×2×1 supercell with the EP localized on Fe4 (-829.858 eV)

0.1777339766124231	0.0122466224558854	0.0858927076448226
0.3257248438889039	0.3099435403607962	0.0824770836978349

0.4870293052070989	0.1674704952116317	0.0843194632833197
0.6805539900557678	0.0141141548087494	0.0844221639152072
0.8372253190903656	0.3202867844864270	0.0857601711880019
0.9853060158143340	0.1649456564010184	0.0839091357572817
0.1802553083969281	0.5126770119058291	0.0842261701483787
0.3326013086060583	0.8200108775343514	0.0844627362299732
0.4836861036143519	0.6689405135342839	0.0850633723829511
0.6934814233235628	0.5155763871555874	0.0820369929064207
0.8309937705495725	0.8180626443395336	0.0834106475005242
0.9909854557785378	0.6698588638832176	0.0830712273635719
0.1569003853857013	0.1741747667838184	0.2589347865356262
0.0154635874061871	0.3419453245709964	0.2589929010328467
0.3469030544236212	0.0030901624894362	0.2503838807193509
0.6555080678825637	0.1530703667584246	0.2509167629631528
0.5015206290390424	0.3480515548918438	0.2499745760963434
0.8473288271267642	-0.0005543451146121	0.2498592341277213
0.1520982028678061	0.6528534843808964	0.2496184176891633
0.0018171321364174	0.8515196157370071	0.2491110497305201
0.3219499576232688	0.4828783030581876	0.2606930578325957
0.6554650851084355	0.6556135123702109	0.2541486095898115
0.4975562707094476	0.8446236017758292	0.2512272700571164
0.8498711512362277	0.4976425989167501	0.2497187053520556
0.0221961394775945	0.1908045988192852	0.4102163960169332
0.3087984112752059	0.3317776786697423	0.4104554240115129
0.1664763339386028	0.4770876013222011	0.4115549088659946
0.5122807167271858	0.1801244873430951	0.4164090604896923
0.8196566498066066	0.3341316642255372	0.4166081136589413
0.6647975462580753	0.4858168996702039	0.4163107293563955
0.0133419585222808	0.6796404783021601	0.4159060525536749
0.3190873912201338	0.8318318725158707	0.4159508238435343
0.1662211195367121	0.9859427308991280	0.4160988692967671
0.5139529272497904	0.6802707320561743	0.4166894729579729
0.8219056344610113	0.8362692490791702	0.417683317859309
0.6676529777105648	0.9879423419917673	0.4165864569322829
0.4838741862305970	0.3200335069704758	0.5812938888265454
0.1794767093239244	0.1658125607487373	0.5822449958292312
0.3332004507006095	0.0136647598484879	0.5821822639057074
0.9862078706229906	0.3202849236310921	0.5824427350592737
0.6802063463497426	0.1667952450502736	0.5823389896387822
0.8358893309480624	0.0160513733825494	0.5813540040976234
0.4861047082489983	0.8196313774219733	0.5824159811963151
0.1798165409985609	0.6641229666923080	0.5810720863131296
0.3341325833121864	0.5137726542094463	0.5826003131323922
0.9867333455869097	0.8192330724308966	0.5830129815947588

0.6805786007052034	0.6672596902363510	0.5831933734464695
0.8325907085259280	0.5134087453217301	0.5828801696514249
0.3468475151824732	0.3467448071459761	0.7495681076535324
0.1531653673973131	-0.0001572799660711	0.7493705316553241
-0.0000069094820706	0.1530337125908730	0.7492204243075056
0.8469719705250045	0.3467077571740642	0.7492484507666762
0.6529868177519141	-0.0003584027183963	0.7492256965056042
0.5003648274915228	0.1535017695429944	0.7493469568649470
0.3467032792928588	0.8470695051195430	0.7491890746711264
0.1533305019569187	0.4996353462812398	0.7493274388466784
0.0006974637629568	0.6533093068948760	0.7492259501069861
0.8464722787736982	0.8469191784051976	0.7494564070913611
0.6529431634744929	0.4997117654512400	0.7495752661642128
0.4997753960606106	0.6530760111779425	0.7498142626798792
0.3195793617691216	0.4859962179128119	0.9171716110735046
0.1659640552519169	0.1795176331230918	0.9157999891538844
0.0132037189420081	0.3325810273571342	0.9166420026569119
0.8211806878494979	0.4857887992607827	0.9154548819637596
0.6672679757828917	0.1798730891141933	0.9169424427679228
0.5147073483927402	0.3338878010687620	0.9170175732079223
0.3202062573841269	0.9869715980896524	0.9169837927315962
0.1672542877245471	0.6803252118023925	0.9163912263902750
0.0140089211088126	0.8337703606707340	0.9164260259999620
0.8193431240100505	0.9860066520300774	0.9166857594132393
0.6661331131648043	0.6798287547739278	0.9170328087116864
0.5132532073146191	0.8334838881816341	0.9167300228801328
0.1664740595327740	0.3317129726351541	0.0213886718546030
0.6687265863016728	0.3328921127247098	0.0217286355441715
0.1687995981433356	0.8362007894630946	0.0210411857414726
0.6637042413745448	0.8322978758930138	0.0215134137635999
-0.0045012013274933	-0.0039323794436389	0.1445334977163295
0.4990338420576688	0.0000447377618987	0.1464504062521990
0.0028271376454009	0.5057197813925189	0.1441670441708691
0.5034484087609175	0.5014290945639424	0.1432892868140428
0.3316984644010867	0.1727759962222096	0.1881729790748996
0.8380068830087549	0.1687256552149073	0.1889807183709042
0.3318786173034127	0.6609219526995436	0.1894092780839375
0.8273989343496854	0.6628352048834616	0.1870245923033743
0.6658856131605569	0.3325838409199168	0.3124835506610689
0.1671454660792875	0.8343172509256779	0.3112966214449820
0.6667027503386769	0.8344847047116496	0.3134395907631050
0.0006713009783853	0.0003263440824013	0.3523474027034266
0.4994495061028253	-0.0001153192362459	0.3534587988794872
-0.0003997418863222	0.4996812304112823	0.3526489502503742

0.4990937730331156	0.5006396905201793	0.3499019251253831
0.3314856099148626	0.1658447793911927	0.4779881730808202
0.8335854879054290	0.1686254366689528	0.4784298038004114
0.3344804027527437	0.6661379842400612	0.4781635140204811
0.8326746532408157	0.6664619229981125	0.4786492942364574
0.1668509562502477	0.3336296098595534	0.5237146679829658
0.6653990193070983	0.3336882627534248	0.5201604361846041
0.1663272384859979	0.8322277542066954	0.5199183540422648
0.6676788691854103	0.8342258034727330	0.5205652203473710
-0.0002207924979276	-0.0008660634800259	0.6460140818241680
0.4998678833258672	0.0000898002985730	0.6456093066604363
-0.0006160134726813	0.5002255657065847	0.6459681764833252
0.5007552692497661	0.5004988404081988	0.6464123483985098
0.3333847810809911	0.1665412898534039	0.6870615421490344
0.8331714835842250	0.1664637195881340	0.6870407558168736
0.3333769884279039	0.6668253046871230	0.6871317813749401
0.8334521387064299	0.6666248711990467	0.6871732288087966
0.1665641003943395	0.3327636148894351	0.8131073735565648
0.6673133159702636	0.3336376724650607	0.8130832817180734
0.1666647256309376	0.8333448563228486	0.8131095844191816
0.6663721226123558	0.8331670799619673	0.8131522419540328
-0.0004673527331883	-0.0003971558137299	0.8539223593015085
0.4999687565407975	0.0003503314376027	0.8541867149909581
0.0013636397302705	0.4998083762745241	0.8537993140495274
0.4996944222248867	0.4996812824938505	0.8547451391184804
0.3336491837385435	0.1682557310578127	0.9802212063306123
0.8334720796600154	0.1658398063319441	0.9800271339419822
0.3330035399907898	0.6666199980492211	0.9805562697862402
0.8337667677853688	0.6651289006642810	0.9788650086675044
0.1654442201454835	0.3330346936483327	0.3211159799651672

(2.5) 2×2×1 supercell with the EP localized on Fe5 (-829.880 eV)

0.1749898735305866	0.0105604745156309	0.0800605276942872
0.3332100033989742	0.3195756142277320	0.0828761675266668
0.4905658668174342	0.1647764132582518	0.0796784185607199
0.6815766018853486	0.0134041330779668	0.0844832756772432
0.8367031555004855	0.3205989047440753	0.0855672613467643
0.9872909778186381	0.1672723914719966	0.0838499928468934
0.1799592817457020	0.5130119513696290	0.0837162523619649
0.3329668881635272	0.8180989804458945	0.0836872185133971
0.4848487355809472	0.6627742969720790	0.0863493540176857
0.6823610131805358	0.5135476748993186	0.0830278430014666
0.8333371091922026	0.8194540425500975	0.0839986379272985
0.9865916951910748	0.6675443963855138	0.0829959319826519

0.1476864832006284	0.1744364462063885	0.2604471357921161
0.0141420403748356	0.3440408832819210	0.2587243044660633
0.3483748509065767	0.9973472001437986	0.2505729119376723
0.6554054329784265	0.1539499570520180	0.2502874475678134
0.5066574548494640	0.3568237069233169	0.2510113249397003
0.8444867249434427	-0.0016124091909230	0.2500751401866345
0.1520450283203845	0.6529977103121594	0.2493567858167030
0.0029713625417543	0.8529092254929669	0.2492144270123525
0.3240933166785914	0.4829358631419587	0.2583713099387243
0.6506733916083230	0.6533852418108618	0.2493956471670369
0.4981868917204742	0.8434083494944589	0.2506418333846933
0.8502098303014195	0.5001381447221671	0.2493657508364977
0.0200483246691153	0.1917637165207022	0.4122517101680744
0.3078258726682321	0.3314244333047779	0.4103212975511544
0.1676174025748681	0.4777466106395591	0.4099088743170074
0.5122338913187904	0.1810273370715581	0.4156109748953336
0.8195438176104152	0.3348469080536384	0.4166662224072407
0.6661101359595714	0.4872855848245221	0.4171637176974179
0.0137167135954361	0.6799528965169844	0.4162330151314590
0.3193027347752936	0.8317396571628692	0.4165043285027640
0.1661334753517443	0.9865157217145826	0.4157708902197823
0.5139859370597955	0.6800629537108380	0.4164910540041009
0.8209297885598269	0.8352954832999312	0.4165854522995212
0.6672733609880840	0.9877210354059732	0.4165761179300499
0.4838767003252981	0.3203083788347044	0.5810161628531708
0.1793187149639815	0.1658423012064220	0.5824095182937112
0.3333777450345398	0.0139095615845950	0.5820906337731873
0.9860413484502283	0.3205822440679532	0.5829856410862603
0.6800409886410146	0.1671621381727293	0.5825561190727822
0.8354449745664240	0.0158673085871387	0.5817578909342702
0.4861828477517010	0.8194444625566851	0.5824227869869296
0.1798383235047869	0.6640151573102939	0.5810488904137977
0.3338196594669841	0.5135117761962227	0.5823731559808378
0.9870076272026900	0.8197226540751096	0.5830625149127401
0.6807572168112483	0.6677722283991480	0.5833112517736296
0.8326948814052703	0.5137097404324245	0.5832067574314400
0.3469543813060654	0.3468926140290334	0.7493201187194803
0.1533697438512192	0.0001439859832305	0.7493341074755745
0.0000659559856838	0.1530971412080002	0.7496827395123471
0.8470186368891590	0.3469208998101743	0.7495611331788055
0.6530241053076629	-0.0006612813284676	0.7495138741703664
0.5003284268712318	0.1532081156856462	0.7491316776776301
0.3470476249968955	0.8468484884783695	0.7490887220960515
0.1533751169759585	0.4997170714118014	0.7494460239556032

0.0005831169143855	0.6530764660752472	0.7492066219131897
0.8467641337253680	0.8470878485639379	0.7496796236978742
0.6529646796173090	0.4997632226298636	0.7496162401905163
0.5000693819799080	0.6531776403119066	0.7498555401349168
0.3200034307026711	0.4868024294097366	0.9165695715455966
0.1677497133071785	0.1806607066136907	0.9164927831295250
0.0136636552038263	0.3328289095971889	0.9166969122444578
0.8206630351158799	0.4864052557384571	0.9164094504179578
0.6690184166818127	0.1801746003582420	0.9157871764888017
0.5144173934799455	0.3331662579921782	0.9164990819098988
0.3198842430946613	0.9858536664855355	0.9159854588152133
0.1670355602178489	0.6797423858268776	0.9163276116917992
0.0128655382362559	0.8319941283404874	0.9151566546725944
0.8199940480468806	0.9854947444231956	0.9171876687061431
0.6659904775404448	0.6796583587359138	0.9172170747652477
0.5138045344832026	0.8331005501838654	0.9176115693072857
0.1676622800683614	0.3331341078386448	0.0206168426661912
0.6686923195693137	0.3318144810989057	0.0207360508327640
0.1677529838297739	0.8340454544835526	0.0199182460771219
0.6648688522324774	0.8315203717081574	0.0228443705748478
0.0028416070323035	0.0021617295866399	0.1452476074203749
0.4991012410454740	0.0010811115749304	0.1455454282456881
0.0023058012612841	0.5040687525225610	0.1448200169258067
0.5012370575709998	0.4931568040780266	0.1453669981422561
0.3257025225688929	0.1631793647146862	0.1901311593288169
0.8371159580576266	0.1673605541154771	0.1892933293834490
0.3318380203937113	0.6621470341033059	0.1891751644994369
0.8334042402998273	0.6688217945881076	0.1874427967266361
0.6656354958381205	0.3339243285141033	0.3115856052288953
0.1681155194607018	0.8344152392390836	0.3120944461847674
0.6658604152691250	0.8333250263517440	0.3127437809582130
0.0003865932117011	0.0033255130704383	0.3525588256089360
0.4995200409972951	-0.0001115208015478	0.3528935850945848
-0.0010369274586082	0.5001383100512730	0.3527414625696106
0.4992817051552298	0.4990042646084344	0.3524335418367287
0.3313855098894778	0.1658399029199179	0.4774864805202190
0.8324208862350821	0.1687699289502382	0.4787328121388341
0.3347536030694979	0.6660505458502975	0.4781337889360198
0.8336337338641009	0.6677425441520658	0.4791136817614263
0.1657851605296727	0.3329000178363098	0.5236455337515016
0.6656979818628909	0.3342955210361581	0.5199130300621473
0.1667658478231884	0.8324520343488707	0.5199500514075205
0.6678157903251493	0.8345903517917109	0.5201187172874452
-0.0004052403695701	-0.0007794259190554	0.6462110258000010

0.4999149015757459	-0.0000449261874546	0.6454233837252134
-0.0006008687896210	0.5004453678723667	0.6461267981287591
0.5007698654578556	0.5007761084258043	0.6460968086170632
0.3335433797256011	0.1667354742897956	0.6867420022788746
0.8331875199537402	0.1665307090051468	0.6873392059461608
0.3334709368287065	0.6665142129450538	0.6870112452852327
0.8333729853629118	0.6667399106692939	0.6872231828517257
0.1669520310274434	0.3330651183788233	0.8129564019299608
0.6667048369350934	0.3331372494107263	0.8128478482020277
0.1669925529924207	0.8334344803308167	0.8123599846139543
0.6668456415050087	0.8330655469295685	0.8134923544133039
0.0008472969098746	0.0005379239263053	0.8543809137632774
0.5005329830840164	-0.0001546477022634	0.8541592645125072
0.0005622515573460	0.4995156318303774	0.8539064756142306
0.4996945672988957	0.4991299277228050	0.8543143184721078
0.3350028960163721	0.1663054401926678	0.9819690389610712
0.8339820817318018	0.1653510874722732	0.9801641712504955
0.3330909123776841	0.6663871269196087	0.9803351385870656
0.8335521228117346	0.6666220958523733	0.9786455368139547
0.1643307367877172	0.3337671097801522	0.3204058505062150

(2.6) 2×2×1 supercell with the EP localized on Fe6 (-829.880 eV)

0.1779254710099554	0.0151515492531778	0.0863495474550737
0.3330528057992288	0.3200409521156660	0.0837163970698150
0.4851322107018072	0.1670334173382063	0.0836871322410241
0.6742108042479664	0.0094344145858947	0.0796784446736427
0.8355707626676611	0.3250103542220753	0.0800606360092510
0.9863657524931130	0.1667902381288480	0.0828761039239697
0.1799815560787743	0.5127091096194049	0.0838499619790252
0.3318276573315078	0.8184234767264043	0.0844832650049225
0.4838958883464290	0.6632967383916902	0.0855673258807789
0.6809531801723617	0.5134085691091909	0.0829957748434544
0.8311867105540630	0.8176391990583587	0.0830280482652942
0.9861172054908294	0.6666632778414976	0.0839985517760890
0.1588426342178686	0.1759066506765389	0.2583714946353186
0.0267501641389282	0.3523132880242434	0.2604473371109898
0.3452213867623742	0.0018131275874089	0.2506417380615457
0.6489720048370998	0.1516248697356139	0.2505728993464638
0.5009527757419346	0.3479549184514243	0.2493566714443570
0.8501662872989019	0.9933426258586074	0.2510116848706403
0.1539008482481710	0.6555132548001825	0.2500750631693189
0.0027117406615813	0.8493266240963989	0.2493956992894391
0.3298989549477955	0.4858581299932550	0.2587244316456660
0.6499283039571605	0.6497900599016321	0.2493657573535829

0.4985445023200375	0.8445944431994549	0.2502874134335090
0.8499378769920405	0.4970287327911340	0.2492142641328896
0.0235985480360880	0.1921741869841797	0.4103214912697764
0.3101289556614891	0.3323823919517653	0.4099089815603735
0.1717153751747032	0.4799514770628917	0.4122518271910863
0.5124366623422056	0.1806971284460837	0.4165040805710629
0.8203819829521251	0.3338662320043400	0.4157705316043053
0.6662360065719493	0.4862828915058685	0.4162328599314349
0.0143657318119159	0.6790699299623862	0.4165854313004344
0.3204474518900015	0.8327263094251106	0.4165761185839392
0.1660767837808274	0.9860136550834886	0.4164910642013819
0.5153029939745605	0.6804558556944630	0.4166662059212298
0.8211754204187670	0.8338897975771514	0.4171636985072645
0.6687932776837343	0.9877658649979812	0.4156108352004306
0.4841765161251100	0.3201614341061247	0.5810487646986555
0.1796919321866526	0.1661801593538597	0.5823730824769003
0.3332615394761015	0.0138169194017186	0.5824228137047334
0.9865234504368369	0.3206812154189880	0.5824093934685007
0.6805315899859589	0.1666219659909012	0.5820904064981940
0.8364316657377414	0.0161231233231637	0.5810161371276351
0.4871211125670408	0.8199589185589469	0.5825561573349213
0.1804223719897396	0.6645549298233561	0.5817578436881438
0.3345407234673087	0.5139584106993182	0.5829857105389190
0.9870148791756725	0.8192425566383716	0.5833113063643278
0.6810147517753957	0.6673049014534999	0.5832067920454901
0.8327147414139171	0.5129920339141282	0.5830624730140264
0.3463420025593639	0.3466246342372097	0.7494459092608660
0.1531082955222004	-0.0000694542602042	0.7498555455549583
-0.0000616929902496	0.1530456806516590	0.7493201186968120
0.8467742102585623	0.3466301876442329	0.7493340271802077
0.6528796412845946	-0.0003283738838348	0.7491317638478926
0.4998008964827921	0.1529522395674538	0.7490885916934783
0.3463147382157566	0.8469760243693942	0.7495139728616536
0.1530313098719658	0.4999339561388227	0.7496827305949719
0.0003236400086486	0.6532357860332504	0.7496795347038907
0.8467985984834331	0.8470351666391824	0.7496162413881409
0.6524933666016351	0.4994169239981999	0.7492065282408591
0.4999024034580377	0.6529814098574068	0.7495611198154706
0.3191653402990162	0.4863364415442694	0.9166969128540735
0.1667991333644208	0.1799968130086836	0.9165695941467900
0.0129110507357977	0.3322503645379930	0.9164929560008152
0.8191288099106776	0.4871346026651732	0.9151565151017372
0.6659696233538651	0.1801160682136540	0.9159854911190946
0.5127069703983951	0.3329647301755583	0.9163275925902670

0.3192961984856121	0.9861957291424562	0.9176115751157747
0.1655006866017195	0.6800061012118644	0.9171876054440025
0.0136682094795768	0.8340099253103360	0.9172170653758793
0.8187489530691399	0.9855827897303777	0.9164992205902566
0.6657424740790135	0.6793371782609355	0.9164094347846987
0.5111562701320659	0.8309817834309295	0.9157873034661500
0.1654718623184259	0.3323378436288489	0.0206169489014296
0.6662929242948326	0.3322473505971748	0.0199181904148988
0.1666519203789387	0.8351315069016227	0.0228444049889969
0.6631223542382042	0.8313082069236644	0.0207361986589041
-0.0080803936239249	-0.0012368159545682	0.1453672106380990
0.5019798382375952	0.0008990621471877	0.1455453368256410
-0.0006795419170441	0.4971589140007788	0.1452474822982155
0.5017634071480760	0.4976942082269579	0.1448199570145895
0.3303088417562344	0.1681619684819172	0.1891753058003217
0.8374768563036726	0.1742976521040076	0.1901313836797765
0.3302447421821572	0.6628839553340137	0.1892934188206685
0.8354175630414417	0.6665959058848779	0.1874427584655251
0.6662998386632023	0.3318844647602849	0.3120942292988726
0.1674642930041026	0.8341393076307337	0.3127436791108495
0.6682888279210853	0.8343644225339653	0.3115855903917926
-0.0002776283617886	0.0007183045548758	0.3524337087288539
0.5003684470860207	0.0004799430934559	0.3528934580628171
0.0029389154368466	0.4996132954666240	0.3525586242685755
0.5011752740130138	0.5010368737379488	0.3527414318582000
0.3312967696175218	0.1652461871769261	0.4781337224353391
0.8344543484515127	0.1686144989834584	0.4774863962131972
0.3363490554405539	0.6675789730237006	0.4787328006431961
0.8341086344949413	0.6663658497447003	0.4791136931456527
0.1671146559561837	0.3342147448067918	0.5236457469150135
0.6656859219395214	0.3332337999242913	0.5199498142123314
0.1667741768253640	0.8321836727868287	0.5201186480472638
0.6685975984009670	0.8343019076229478	0.5199130037534514
0.0000062132462140	-0.0007701662538638	0.6460968656249017
0.5000401618121046	0.0000849817858229	0.6454232772686248
-0.0003743378498426	0.5004051415211849	0.6462110664615000
0.5010460840572299	0.5006005678895250	0.6461267331760854
0.3330431105714865	0.1665289233184269	0.6870112038713142
0.8331921363832491	0.1664565081894633	0.6867419383054991
0.3333429534867037	0.6668121406784637	0.6873392475770530
0.8333667660201549	0.6666269656712349	0.6872231412814827
0.1661131926880945	0.3330479958585030	0.8129563978342789
0.6664421026803177	0.3330074221305129	0.8123599974480278
0.1662199406351898	0.8331542628900308	0.8134924914237990

0.6664324406011838	0.8332952893133013	0.8128480560052086
-0.0005646340972041	0.0003056445301202	0.8543143826876436
0.4993126351290447	-0.0005327080443402	0.8541593725155899
-0.0003092232307878	0.4991526970527648	0.8543808844398877
0.4989536419054743	0.4994380798771836	0.8539064915833593
0.3332967892050405	0.1669095419018020	0.9803351850119979
0.8313025355385238	0.1649971236660367	0.9819691842075861
0.3313689719369503	0.6660181941619870	0.9801641805635373
0.8330702193885985	0.6664482215612586	0.9786453969351679
0.1694361993251740	0.3356693280671835	0.3204059823370376

(2.7) $2\times2\times1$ supercell with the EP localized on Fe7 (-829.879 eV)

0.1793430297835232	0.0159812819431974	0.0855864564050615
0.3327088610657294	0.3198867713191930	0.0838239717841703
0.4865945210174973	0.1680919536928242	0.0845103790376145
0.6818205716985719	0.0147333223349237	0.0837479908228453
0.8371680482473264	0.3220213395809597	0.0864041933478914
0.9868832624027958	0.1668880289526737	0.0836923968425444
0.1804943072419410	0.5135632636645882	0.0829131115276746
0.3351321246519354	0.8257125381501267	0.0797487523432306
0.4894336253014528	0.6643840928275357	0.0801414204068724
0.6805156687079706	0.5137614448936932	0.0840033650358914
0.8324279255733715	0.8189426551757933	0.0830112683387952
0.9864141835157267	0.6687091299604339	0.0830468511305931
0.1558990623727785	0.1701812869429325	0.2586654278441906
0.0171377403697591	0.3413834164940590	0.2582535053711768
0.3460922652353098	0.0015627665618904	0.2503017466519284
0.6566593090847623	0.1548393113982131	0.2506644240155771
0.5016441537670288	0.3461606034651065	0.2500431998230404
0.8470388738147654	-0.0009017645422366	0.2493352707188716
0.1432014989390879	0.6499829697607330	0.2509928305106094
-0.0001516145677507	0.8501377954179002	0.2494175308469260
0.3256350080916700	0.4732648879989406	0.2603262890456435
0.6470499609032252	0.6500929134636801	0.2492444231584677
0.5026480080736623	0.8510712821478539	0.2506144881108305
0.8466456197722720	0.4973402412593869	0.2494466003493346
0.0222487988440801	0.1900253587863953	0.4098058237817300
0.3082879708901565	0.3284145677469170	0.4122247064473978
0.1685973980607066	0.4765590966163571	0.4102409585030347
0.5123293279323351	0.1796575753883691	0.4165600517300366
0.8200141734703269	0.3341308316441986	0.4164836678381246
0.6648318395373977	0.4858397575670521	0.4165601841945618
0.0127408022757872	0.6790159113140196	0.4171607070243585
0.3190372723596530	0.8313788772754900	0.4156718856277226

0.1651717955990118	0.9848302797702885	0.4166542985258898
0.5135676492475254	0.6797177421860767	0.4157960745387846
0.8200993873884499	0.8338675307549834	0.4162546314929642
0.6682724575260730	0.9876542489291110	0.4165324382428827
0.4841645774893389	0.3197077950215233	0.5816893695360822
0.1794383511320118	0.1655291202031209	0.5829177800194367
0.3329502702270964	0.0129551668125028	0.5825173471752016
0.9865217988450702	0.3204129218396102	0.5822801336521345
0.6805388154033797	0.1667956806322021	0.5823924915338347
0.8361010122979653	0.0159608709417697	0.5810365065249312
0.4861762093131457	0.8196083561437584	0.5821018695178393
0.1797391020201962	0.6636298040638199	0.5810067689643842
0.3342329602551977	0.5136321177922823	0.5823517799773167
0.9863553881866199	0.8190363913818843	0.5832417443777909
0.6803805703599262	0.6674460125785430	0.5831061630031796
0.8322501807562953	0.5130852207083976	0.5833020270081465
0.3469025910858640	0.3469232230690486	0.7496493824380959
0.1531044540213030	0.0000571237843005	0.7495859284379358
0.0001891126460822	0.1535302353587451	0.7494557185471644
0.8467926550796497	0.3468317919241119	0.7498377353174982
0.6532196630653277	0.0001243575453257	0.7490878500670002
0.5006277981253849	0.1536587191325056	0.7494638083501142
0.3467324940560737	0.8470099697286153	0.7491301596799068
0.1530433799470362	0.5000146084949652	0.7492707853527112
0.0002484149256665	0.6531675203547477	0.7496306247346617
0.8468609513289037	0.8474324167225533	0.7492390188256406
0.6528988931279990	0.4995633671160712	0.7496530074675397
0.4997843646066135	0.6531141220874813	0.7493762429468711
0.3192696407519507	0.4869315400386632	0.9164791426795174
0.1670890347401552	0.1807019919236500	0.9166644334598278
0.0131451176515084	0.3330761571909521	0.9165606800787310
0.8202921668823903	0.4861484540520888	0.9172325144950203
0.6667641150106035	0.1804829106259778	0.9176661849564186
0.5144367745017885	0.3343507269623048	0.9171937750757864
0.3198102891552934	0.9886748360222930	0.9158404345459854
0.1667241672738096	0.6810817839555479	0.9165776043522401
0.0135424204493402	0.8341365039644283	0.9164419234414580
0.8202191046406174	0.9871142388635038	0.9164113126325543
0.6679208457428787	0.6806461385291578	0.9152112419317439
0.5140905374705007	0.8339521734520186	0.9160511590612179
0.1667949493461420	0.3343845285600273	0.0205944506695122
0.6684659742193875	0.3332182864965100	0.0228367459255172
0.1680813753104725	0.8367387629470326	0.0207637196432472
0.6659397152848849	0.8336055975134969	0.0199406996395978

-0.0041143116803176	-0.0018654602826749	0.1448356025683840
0.4988412483816526	-0.0020704033857797	0.1455890546486298
0.0069132184854452	0.5080021116042382	0.1454292967489601
0.4978576729771905	0.5006343228162780	0.1452383182969889
0.3326490157446460	0.1698239054204108	0.1892525848778126
0.8378405833100532	0.1697309229794765	0.1891234099790431
0.3368218643868890	0.6624965401000090	0.1901633749839476
0.8311680462553753	0.6645748725344066	0.1874864033576825
0.6666773155445914	0.3325531753900978	0.3127534982194226
0.1661585818187944	0.8318886166923736	0.3116017858712145
0.6656062848282486	0.8338023772429541	0.3121293955961040
-0.0000279290170044	-0.0010211949869947	0.3527437118123151
0.5001867518295315	-0.0002271253201307	0.3529256499810610
0.0010139802874517	0.5004692099805576	0.3524458052261363
0.4967645932227407	0.4972167208173339	0.3525501000252259
0.3312781505286772	0.1637670925112142	0.4786919160584887
0.8339924606573178	0.1688980020237323	0.4780927333492260
0.3342910500004331	0.6657309632540368	0.4774731303836753
0.8322967169932628	0.6660470603917528	0.4791095126631723
0.1671873816525581	0.3330451902144048	0.5235450351085738
0.6654572740814920	0.3333431294829006	0.5201285925064935
0.1657593856629608	0.8315174532344195	0.5199478049341090
0.6676413140123221	0.8344663506411846	0.5200025194462899
-0.0004469147922021	-0.0010075405801544	0.6461128697161443
0.5000820769307961	0.0000016394413052	0.6454763028172091
-0.0006973081962564	0.5001086700173587	0.6460406758273908
0.5008289405194543	0.5004100429484587	0.6461662064238664
0.3334496540222247	0.1665990913397310	0.6872694729455189
0.8334506059035721	0.1669538244303330	0.6869495227754855
0.3332837870928175	0.6667995855850669	0.6867007113677890
0.8332731373400224	0.6666031145900256	0.6872729650686361
0.1668677061584054	0.3337673662883190	0.8129338429080865
0.6668977754070252	0.3336716667705420	0.8134539709530845
0.1668112567846168	0.8334719181295440	0.8128749628244780
0.6665292763335738	0.8334293553159258	0.8124098921736811
0.0004332657701792	0.0009027615347963	0.8539016686337523
0.5000838113923267	0.0005232078365113	0.8541366104875682
0.0008067708277380	0.5003987311367636	0.8542780626668071
0.4993686166048157	0.5001545011893463	0.8543682301157023
0.3345198961238278	0.1684836404092038	0.9801541097343190
0.8335804247832005	0.1666301850406780	0.9803588508559977
0.3336234019315528	0.6684992297539692	0.9820288944632352
0.8332936981694790	0.6667238469573429	0.9787377787332777
0.1662248209987603	0.3306956481295514	0.3202951944039795

(2.8) $2 \times 2 \times 1$ supercell with the EP localized on Fe8 (-829.919 eV)

0.1801768215589934	0.0160324124832275	0.0849584718344283
0.3337266406651093	0.3204396733891730	0.0844748708440609
0.4861758768055737	0.1665753141659380	0.0838403820549396
0.6809296296884763	0.0134813496955483	0.0841621450045210
0.8362891022226434	0.3198861248951444	0.0850135337845208
0.9869218614391830	0.1657040131711665	0.0843532715868267
0.1803206530847336	0.5130065512718365	0.0840678909529123
0.3337682994042581	0.8193943850576622	0.0839256315315530
0.4843374625618171	0.6642070079642804	0.0851187685578643
0.6772878793982066	0.5088819262916081	0.0783389359352356
0.8309842288886583	0.8177624921873576	0.0828080086522986
0.9914748180284163	0.6673610443018771	0.0789059043685146
0.1589514512759549	0.1764291426249895	0.2591610218747016
0.0161601471889467	0.3414747075347520	0.2589933650220093
0.3481090062350332	0.0039921518347366	0.2505961455139135
0.6557065899274300	0.1526745253665213	0.2506205488103115
0.5017715061583004	0.3484828864816864	0.2491569845678300
0.8462150236822317	-0.0013089819197460	0.2495021113544139
0.1517587576961810	0.6536324372743476	0.2489186363710547
0.0099713645015799	0.8623270742327610	0.2502403295104332
0.3227605646904623	0.4830287966504351	0.2597054816334351
0.6359476713552408	0.6489468185768176	0.2510273045410145
0.4963171470343166	0.8450526729105241	0.2509242551188678
0.8502890965483061	0.4930379582202745	0.2492801622573451
0.0223813668327089	0.1911033731766002	0.4104250025858397
0.3087480120668954	0.3319767592281586	0.4109181104872057
0.1672962462524762	0.4775370648170137	0.4108796644425807
0.5125177329432870	0.1806385523596874	0.4162351756253340
0.8196426414931276	0.3338212313796540	0.4168422979411882
0.6654717058373883	0.4864574643454750	0.4156067567200335
0.0135129990043725	0.6798584881509731	0.4154001502790568
0.3194437155321986	0.8323355934358325	0.4162798011289350
0.1669060217720507	0.9866277302399942	0.4174099909662939
0.5132062190375692	0.6806761676266143	0.4180543391367623
0.8201424226098381	0.8343078710917672	0.4159085218828664
0.6674815282297709	0.9877941683512154	0.4165505104524819
0.4844104105334910	0.3203820289706850	0.5812704508667882
0.1796805220856288	0.1661980981937190	0.5827803805765562
0.3333312655853428	0.0139165887622854	0.5825438949653752
0.9862427940608429	0.3202243941947867	0.5826372731974971
0.6804916264968582	0.1668666383800175	0.5824577437592402
0.8359560208118290	0.0157803121004550	0.5811928637088328
0.4860599277865959	0.8196217693526668	0.5828461192085442

0.1795705739222680	0.6642799316547197	0.5812280402648071
0.3336373791257866	0.5135725935984461	0.5829192594196231
0.9865172341080704	0.8194208895220028	0.5828168604906543
0.6805744998139734	0.6672357510886691	0.5830076461765696
0.8328160331431462	0.5135202955834061	0.5827540418605103
0.3467364822785419	0.3469189300483954	0.7495284680212083
0.1532866447565070	0.0001726451063792	0.7496449854301973
0.0002083485583328	0.1532987445764940	0.7497031657923053
0.8470905993454636	0.3467092549328718	0.7494232890435163
0.6532162268410088	-0.0004008864413197	0.7494003237744480
0.5005404574438851	0.1532438176750847	0.7490912439825791
0.3468767597734065	0.8472292286285297	0.7492465504000742
0.1531759664798474	0.4996425055319373	0.7495107310852248
0.0003677086857492	0.6532174112632396	0.7492660723868914
0.8469715820308031	0.8472246317366041	0.7493925433129863
0.6529680838753383	0.4998107945104341	0.7493029612547480
0.4999447798166224	0.6531198245291856	0.7498341872407290
0.3199587935793985	0.4862653407287665	0.9170708200627278
0.1669619818896884	0.1804430958753694	0.9170338694697608
0.0138874374382325	0.3331282424834201	0.9171436751560380
0.8201693345902941	0.4854687063691330	0.9157873603878159
0.6674026864397848	0.1794073284711445	0.9167084400850697
0.5130150769411956	0.3317707934250128	0.9153085287749920
0.3204939595007052	0.9873708414952144	0.9166827125080105
0.1684661228235197	0.6808330241407355	0.9153468784232526
0.0141423067362835	0.8339108172866986	0.9164590225597116
0.8198408058124627	0.9862067603180821	0.9166431794277852
0.6668354442078388	0.6802138535424453	0.9165381672430735
0.5134196507970089	0.8330333155101841	0.9169513824602158
0.1669730349834599	0.3328928849468246	0.0218334064879577
0.6675302929033469	0.3304693552773451	0.0202064852485041
0.1692799414568270	0.8363340033567157	0.0206284316563183
0.6647238264096309	0.8319335129849825	0.0212279155812700
-0.0054701922831384	-0.0063738947411387	0.1448661126127623
0.5000112530153922	-0.0000046276859038	0.1464764375815939
0.0014838648034878	0.5063357382777683	0.1431825405479479
0.5078350606439354	0.5006527608788320	0.1441147128064753
0.3307470334722019	0.1706630940179342	0.1891962550520143
0.8391874996426093	0.1690886666696700	0.1892471409651761
0.3306301345315989	0.6607245985316508	0.1895289651630361
0.8287337198156601	0.6617095350090978	0.1894180014967858
0.6668479010501692	0.3325441053191421	0.3121153216703995
0.1672245452329229	0.8353384913842196	0.3115035113467264
0.6651312541811223	0.8333091303482343	0.3125799397031124

0.0014027123158474	0.0006753137937559	0.3524104653605393
0.4996063601265303	0.0000153660849452	0.3537121012023208
-0.0005709126474376	0.4993103347996853	0.3518967250225940
0.4982125789447385	0.5012191348615880	0.3525707623646644
0.3320773181512707	0.1662298177400058	0.4784733656295072
0.8338218875285532	0.1683165276401642	0.4782946183186941
0.3334437380394436	0.6662312184367498	0.4786509632346675
0.8330800849728275	0.6667738310637638	0.4780935106962713
0.1666109050790117	0.3334381466443198	0.5237350748185693
0.6660110258803054	0.3337409269752804	0.5199543758239867
0.1664302954467327	0.8327610537993879	0.5198399478981681
0.6672076857602216	0.8339713807670862	0.5202798004608655
-0.0001909452453715	-0.0007689771389965	0.6461177375597033
0.5000266002680036	0.0001909174947020	0.6455314957932373
-0.0006745324800883	0.5001622431384042	0.6459995811524653
0.5006618635788698	0.5006442112043900	0.6461939365902998
0.3334767912434308	0.1667294151774219	0.6871980446472087
0.8333406005361969	0.1664172416118884	0.6871295463005185
0.3333676484907845	0.6668075133206444	0.6872875735802010
0.8334291045628978	0.6667953918626959	0.6867930491072574
0.1668964799463953	0.3332970795776403	0.8132258059464098
0.6670828271013440	0.3336329653253120	0.8125202832512676
0.1664926646231378	0.8331715460219487	0.8128027644313797
0.6669577865145346	0.8330878539644355	0.8130923404367932
0.0003287288201935	0.0001605814191586	0.8542542137343105
0.5002098831924213	-0.0001706852975981	0.8539166804012618
0.0008037308669249	0.4998645172585481	0.8540365154657537
0.5001618603545834	0.4998975064268694	0.8543652327134930
0.3343625301385121	0.1678652306543350	0.9801528714961960
0.8339870693375608	0.1655964101942914	0.9803381908694977
0.3327706047801862	0.6664594781771475	0.9801097947478871
0.8341501985042896	0.6656041610644491	0.9806571089038582
0.1657883966404600	0.3333589043484189	0.3210143500101547

(2.9) $2\times 2\times 1$ supercell with the EP transfer from Fe1 to Fe5 as an example

Initial coordinate: 0 (-829.858 eV)

0.1852597094262997	0.0163100845483613	0.0850694260350203
0.3324235780448301	0.3197457251547390	0.0842269381227621
0.4874127121802198	0.1674006641282402	0.0844637035981047
0.6804381314677047	0.0129713147209025	0.0843166417247695
0.8345126560043925	0.3222669409531168	0.0858925866834335
0.9842134267051003	0.1742717440001440	0.0824769107959521
0.1796393556952068	0.5146913700196987	0.0839090020926492
0.3335623519170481	0.8194440412252807	0.0844222164454812

0.4830621704847896	0.6627739334316222	0.0857586609344587
0.6788741452968879	0.5090208928575554	0.0830729876144729
0.8221001582668690	0.8065231084279444	0.0820357530872148
0.9870668214175093	0.6690029137840428	0.0834114314414733
0.1609262305293208	0.1780515570189322	0.2606859907112975
0.0172803931496926	0.3431062874581790	0.2589295622242428
0.3470689353999330	0.0024447267617426	0.2512297207044198
0.6561877735764262	0.1530950670743975	0.2503867406229499
0.5007622968178487	0.3479052769934449	0.2496203220828493
0.8465231473835113	-0.0015239896155017	0.2499705064626469
0.1521183261370685	0.6526721878486135	0.2498585425885110
0.0001473718543373	0.8445292946871839	0.2541458585068425
0.3264848284295498	0.4845351301665262	0.2589878380040375
0.6477726909342889	0.6501333913881768	0.2497191511584183
0.4975598325693182	0.8444923776873520	0.2509179481394150
0.8497001753467341	0.4981824676421842	0.2491123329445500
0.0229769852850704	0.1912021667818427	0.4104499111519438
0.3106115204699557	0.3335229685481999	0.4115526385300805
0.1686123056436227	0.4778058468589493	0.4102138249087040
0.5127489303613528	0.1809130445051836	0.4159534028532043
0.8197227122503857	0.3337798406960159	0.4160998520593993
0.6662982075002024	0.4866577633083360	0.4159089237664717
0.0143628529405047	0.6780928455171391	0.4176831558751842
0.3202867705086996	0.8323483922274439	0.4165874367539736
0.1663146159325015	0.9860454580958760	0.4166863011428058
0.5144753871840074	0.6803435112186679	0.4166094471610683
0.8210187325052316	0.8352055986330826	0.4163099129971857
0.6678379171466110	0.9877155640262324	0.4164110521394014
0.4843057362555999	0.3201831636418789	0.5810728524645407
0.1796383710354916	0.1658656799809513	0.5825982408057737
0.3335249313013355	0.0138929077571194	0.5824169314537059
0.9863371479897197	0.3205238096252156	0.5822433446127732
0.6804645062232941	0.1668001130365180	0.5821858596420810
0.8361599893337908	0.0161252202194075	0.5812929458364964
0.4865863140719502	0.8197922337701096	0.5823418992320442
0.1801601593604236	0.6641084119562678	0.5813533889796640
0.3340753516381485	0.5137915085522401	0.5824425355480087
0.9866791644459112	0.8194211974354337	0.5831929318754069
0.6808184859180041	0.6674093912031164	0.5828812867245550
0.8325004186712093	0.5132675650452145	0.5830156224180287
0.3463042674428694	0.3466687723687629	0.7493288017791985
0.1533001220614189	0.0002227405122298	0.7498154513307782
-0.0001002203459345	0.1531533621953271	0.7495679646909822
0.8466775244241891	0.3468348939769526	0.7493719140091248

0.6531349111005702	-0.0003653092403689	0.7493470966576714
0.5003661321747044	0.1532957151415706	0.7491901638635408
0.3466532805426753	0.8470143721539104	0.7492267210280978
0.1530401762720148	0.5000054252570589	0.7492207964649508
0.0004467124429329	0.6535285143017134	0.7494572718915730
0.8467685137661798	0.8470559565238852	0.7495751757425139
0.6526129260627510	0.4993036588309076	0.7492265763397737
0.4997363231869868	0.6530291423617062	0.7492484288531971
0.3193783526806735	0.4867939392985325	0.9166424290780412
0.1664165462536026	0.1804177908152376	0.9171755170391884
0.0135523465397541	0.3340360697784153	0.9158007139495529
0.8197620556611859	0.4859940904832837	0.9164262576578807
0.6667648482262133	0.1797968604171060	0.9169816143611147
0.5130708201677685	0.3327463003166740	0.9163924694466520
0.3202308102648387	0.9867444705718618	0.9167312927212005
0.1666640423395184	0.6806551035914404	0.9166855770756800
0.0136974091667441	0.8338669250069451	0.9170338095662424
0.8191779810320085	0.9852943060375445	0.9170153669320157
0.6646096875862112	0.6788213749951221	0.9154534797707913
0.5126038460207729	0.8327299635661626	0.9169397631231042
0.1652372378865681	0.3335203558346036	0.0213867137627135
0.6673991382143475	0.3312079258371842	0.0210428259311438
0.1685924131063290	0.8362895819113599	0.0215161630928898
0.6641737236351090	0.8312800310310997	0.0217274886657116
-0.0020049914341373	-0.0034376730164282	0.1432827346604270
0.5010112344057719	0.0009661955421873	0.1464513967574395
0.0005692853985496	0.5044968731080589	0.1445333773207509
0.5028887244201257	0.4971756123975759	0.1441681834095554
0.3290551742898880	0.1681282200200310	0.1894116401768411
0.8410716208176284	0.1682949802914738	0.1881724594336167
0.3307185238996527	0.6619982358434982	0.1889796916852459
0.8354328381919540	0.6725974292558811	0.1870274554891828
0.6671723529861532	0.3328509959378916	0.3113034006670586
0.1677803374496027	0.8332960263389807	0.3134409608884815
0.6666966898258446	0.8341171543477491	0.3124870697813440
0.0015420830675765	0.0009051121981949	0.3498943992124922
0.5004312900593437	0.0005508805605507	0.3534577940519070
-0.0003456663846943	0.4993295264213302	0.3523481403858594
0.5000850314464163	0.5004012481472699	0.3526509168426095
0.3316567876054387	0.1655192347468392	0.4781617574377575
0.8343585179054288	0.1685093077861091	0.4779872815521404
0.3350351605136452	0.6664135540715381	0.4784283916195142
0.8337860737979098	0.6673274504270462	0.4786498759296215
0.1667788219417419	0.3331480513392982	0.5237098024303231

0.6659016440231965	0.3336717113049547	0.5199221531026779
0.1665452960704009	0.8323232318435297	0.5205652055403264
0.6682837613987619	0.8345977070237646	0.5201626448390084
-0.0002562031504752	-0.0007557438541711	0.6464132840078681
0.5002196740676007	0.0001322283835436	0.6456083983514427
-0.0006450950374784	0.5002182613243188	0.6460147814989758
0.5008392950272436	0.5006156348444358	0.6459687475219964
0.3334473407703586	0.1666238346382275	0.6871309050945629
0.8331596386133476	0.1666156444199299	0.6870612005921588
0.3332904241981375	0.6668271613070692	0.6870415703713827
0.8331737964518510	0.6665477804015076	0.6871722212084670
0.1661996997978152	0.3334351474792982	0.8131082374223362
0.6666790346455906	0.3333341035754428	0.8131097356115672
0.1667947695619371	0.8336275637885986	0.8131534538762819
0.6663246095516279	0.8326880561651469	0.8130817023394734
-0.0000138002985834	0.0003051233616631	0.8547469773156974
0.5003804878043511	0.0000308672801681	0.8541879511380644
0.0000698952226920	0.5004675326937548	0.8539227211916349
0.4984486293474411	0.4986376677811525	0.8537989721317238
0.3336192221166527	0.1669933269960238	0.9805582029094255
0.8346024125185235	0.1663515414030890	0.9802197888600864
0.3323698045148429	0.6665263004212161	0.9800257412582107
0.8313658329457239	0.6662378518085499	0.9788651543396157
0.1675931087137136	0.3345558339641834	0.3211092952610840

Interpolating coordinate: 0.167 (-829.841 eV)

0.183548070	0.015351816	0.084234610
0.332554649	0.319717373	0.084001810
0.487938238	0.166963289	0.083666156
0.680627877	0.013043451	0.084344414
0.834877739	0.321988935	0.085838366
0.984726352	0.173105185	0.082705758
0.179692677	0.514411467	0.083876877
0.333463108	0.819219864	0.084299717
0.483359931	0.662773994	0.085857110
0.679455290	0.509775357	0.083065464
0.823972983	0.808678264	0.082362901
0.986987634	0.668759828	0.083342182
0.158719606	0.177449039	0.260646182
0.016757334	0.343262053	0.258895353
0.347286588	0.001595139	0.251120253
0.656057383	0.153237549	0.250370192
0.501744823	0.349391682	0.249852156
0.846183744	-0.001538726	0.249987945

0.152106110	0.652726442	0.249774916
0.000618037	0.845925950	0.253323953
0.326086243	0.484268586	0.258885083
0.648256141	0.650675366	0.249665234
0.497664342	0.844311706	0.250871929
0.849785118	0.498508414	0.249154569
0.022488875	0.191295758	0.410750211
0.310147246	0.333173213	0.411347415
0.168446488	0.477795974	0.410163000
0.512663091	0.180932093	0.415896332
0.819692896	0.333957685	0.416194247
0.666266862	0.486762400	0.416118056
0.014255163	0.678402854	0.417441466
0.320122765	0.832246936	0.416573585
0.166284426	0.986123835	0.416533733
0.514393812	0.680296752	0.416589715
0.821003909	0.835220579	0.416355836
0.667743824	0.987716476	0.416438563
0.484234230	0.320204033	0.581063404
0.179585095	0.165861784	0.582566787
0.333500400	0.013895683	0.582362549
0.986287848	0.320533549	0.582367061
0.680393920	0.166860451	0.582247570
0.836040820	0.016082235	0.581370437
0.486519070	0.819734272	0.582355381
0.180106520	0.664092870	0.581302639
0.334032736	0.513744886	0.582430972
0.986733908	0.819471440	0.583171196
0.680808274	0.667469864	0.582952948
0.832532829	0.513341261	0.583047478
0.346412620	0.346706079	0.749327355
0.153311726	0.000209615	0.749735227
-0.000072524	0.153143992	0.749587094
0.846734377	0.346849228	0.749403451
0.653116443	-0.000414638	0.749374893
0.500359848	0.153281115	0.749180416
0.346719005	0.846986725	0.749203721
0.153096000	0.499957366	0.749258334
0.000469447	0.653453173	0.749415497
0.846767784	0.847061272	0.749592584
0.652671552	0.499380253	0.749291520
0.499791833	0.653053892	0.749349614
0.319482532	0.486795354	0.916630286
0.166638741	0.180458277	0.917061728

0.013570898	0.333834876	0.915950080
0.819912219	0.486062618	0.916423456
0.667140443	0.179859817	0.916782541
0.513295249	0.332816293	0.916410238
0.320173049	0.986596003	0.916606987
0.166725962	0.680502984	0.916625916
0.013558764	0.833554792	0.916720950
0.819313992	0.985327712	0.917044084
0.664839819	0.678960872	0.915747412
0.512803961	0.832791728	0.917051731
0.165641412	0.333455981	0.021258402
0.667614668	0.331309018	0.020991697
0.168452508	0.835915561	0.021249844
0.664289578	0.831320088	0.021913636
-0.001197225	-0.002504439	0.143610213
0.500692902	0.000985348	0.146300402
0.000858705	0.504425520	0.144581151
0.502613447	0.496505811	0.144367986
0.328496399	0.167303411	0.189531560
0.840412344	0.168139243	0.188359271
0.330905107	0.662023036	0.189012270
0.835094739	0.671968157	0.187096679
0.666916210	0.333029885	0.311350435
0.167836201	0.833482562	0.313216542
0.666557311	0.833985133	0.312529855
0.001349501	0.001308512	0.350338470
0.500279415	0.000440480	0.353363759
-0.000460877	0.499464324	0.352413694
0.499951144	0.500168418	0.352614688
0.331611575	0.165572679	0.478049211
0.834035579	0.168552745	0.478111537
0.334988234	0.666353053	0.478379291
0.833760684	0.667396633	0.478727177
0.166613212	0.333106712	0.523699091
0.665867700	0.333775680	0.519920633
0.166582055	0.832344699	0.520462680
0.668205766	0.834596481	0.520155324
-0.000281043	-0.000759691	0.646379574
0.500168879	0.000102703	0.645577563
-0.000637724	0.500256112	0.646033451
0.500827723	0.500642380	0.645990091
0.333463347	0.166642441	0.687066088
0.833164286	0.166601489	0.687107535
0.333320510	0.666775003	0.687036516

0.833206995	0.666579802	0.687180715
0.166325088	0.333373476	0.813082932
0.666683335	0.333301295	0.813066088
0.166827733	0.833595383	0.813021209
0.666411448	0.832750971	0.813150144
0.000129716	0.000343923	0.854685967
0.500405904	-0.000000052	0.854183170
0.000151955	0.500308883	0.853920014
0.498656286	0.498719711	0.853884863
0.333849834	0.166878679	0.980793342
0.834499024	0.166184799	0.980210519
0.332489989	0.666503105	0.980077307
0.831730215	0.666301892	0.978828551
0.167049380	0.334424380	0.320992054

Interpolating coordinate: 0.333 (-829.791 eV)

0.181836431	0.014393548	0.083399793
0.332685720	0.319689022	0.083776681
0.488463764	0.166525914	0.082868609
0.680817622	0.013115588	0.084372186
0.835242823	0.321710929	0.085784145
0.985239277	0.171938626	0.082934605
0.179745998	0.514131564	0.083844752
0.333363864	0.818995688	0.084177217
0.483657692	0.662774055	0.085955559
0.680036435	0.510529820	0.083057939
0.825845809	0.810833420	0.082690048
0.986908446	0.668516741	0.083272932
0.156512981	0.176846520	0.260606372
0.016234276	0.343417819	0.258861143
0.347504241	0.000745551	0.251010784
0.655926993	0.153380030	0.250353643
0.502727349	0.350878087	0.250083990
0.845844340	-0.001553463	0.250005384
0.152093894	0.652780695	0.249691290
0.001088702	0.847322605	0.252502048
0.325687658	0.484002041	0.258782329
0.648739591	0.651217342	0.249611316
0.497768852	0.844131035	0.250825910
0.849870060	0.498834360	0.249196806
0.022000765	0.191389350	0.411050511
0.309682971	0.332823457	0.411142192
0.168280671	0.477786101	0.410112175
0.512577251	0.180951142	0.415839260

0.819663081	0.334135530	0.416288642
0.666235517	0.486867037	0.416327188
0.014147473	0.678712863	0.417199776
0.319958759	0.832145481	0.416559734
0.166254236	0.986202213	0.416381164
0.514312237	0.680249992	0.416569983
0.820989085	0.835235560	0.416401759
0.667649732	0.987717388	0.416466074
0.484162724	0.320224902	0.581053956
0.179531819	0.165857887	0.582535333
0.333475869	0.013898459	0.582308166
0.986238548	0.320543288	0.582490777
0.680323334	0.166920788	0.582309279
0.835921651	0.016039250	0.581447928
0.486451825	0.819676310	0.582368862
0.180052881	0.664077327	0.581251889
0.333990121	0.513698264	0.582419409
0.986788652	0.819521683	0.583149460
0.680798063	0.667530337	0.583024608
0.832565240	0.513414957	0.583079334
0.346520972	0.346743386	0.749325907
0.153323329	0.000196489	0.749655003
-0.000044828	0.153134622	0.749606223
0.846791229	0.346863563	0.749434987
0.653097976	-0.000463967	0.749402689
0.500353564	0.153266515	0.749170668
0.346784729	0.846959078	0.749180721
0.153151823	0.499909307	0.749295872
0.000492181	0.653377832	0.749373722
0.846767054	0.847066587	0.749609992
0.652730177	0.499456847	0.749356464
0.499847343	0.653078642	0.749450799
0.319586712	0.486796769	0.916618143
0.166860935	0.180498763	0.916947939
0.013589449	0.333633683	0.916099447
0.820062382	0.486131146	0.916420655
0.667516038	0.179922774	0.916583468
0.513519678	0.332886286	0.916428007
0.320115288	0.986447536	0.916482681
0.166787882	0.680350864	0.916566255
0.013420119	0.833242659	0.916408091
0.819450003	0.985361119	0.917072801
0.665069951	0.679100370	0.916041345
0.513004076	0.832853492	0.917163699

0.166045585	0.333391607	0.021130090
0.667830199	0.331410111	0.020940568
0.168312603	0.835541539	0.020983524
0.664405433	0.831360145	0.022099783
-0.000389459	-0.001571205	0.143937692
0.500374570	0.001004501	0.146149407
0.001148124	0.504354166	0.144628924
0.502338169	0.495836010	0.144567788
0.327937624	0.166478602	0.189651480
0.839753067	0.167983505	0.188546083
0.331091689	0.662047835	0.189044849
0.834756639	0.671338884	0.187165903
0.666660067	0.333208773	0.311397469
0.167892065	0.833669097	0.312992123
0.666417932	0.833853112	0.312572640
0.001156920	0.001711912	0.350782541
0.500127540	0.000330080	0.353269724
-0.000576087	0.499599121	0.352479248
0.499817256	0.499935587	0.352578459
0.331566362	0.165626124	0.477936665
0.833712641	0.168596182	0.478235792
0.334941308	0.666292551	0.478330191
0.833735294	0.667465815	0.478804478
0.166447601	0.333065374	0.523688380
0.665833757	0.333879648	0.519919112
0.166618813	0.832366166	0.520360154
0.668127771	0.834595255	0.520148002
-0.000305882	-0.000763638	0.646345865
0.500118083	0.000073177	0.645546727
-0.000630353	0.500293964	0.646052120
0.500816152	0.500669126	0.646011435
0.333479354	0.166661048	0.687001271
0.833168932	0.166587333	0.687153869
0.333350595	0.666722845	0.687031462
0.833240193	0.666611824	0.687189208
0.166450477	0.333311804	0.813057626
0.666687635	0.333268486	0.813022440
0.166860697	0.833563203	0.812888964
0.666498287	0.832813886	0.813218586
0.000273232	0.000382724	0.854624956
0.500431320	-0.000030971	0.854178389
0.000234014	0.500150232	0.853917306
0.498863942	0.498801754	0.853970754
0.334080447	0.166764031	0.981028482

0.834395636	0.166018057	0.980201250
0.332610174	0.666479909	0.980128874
0.832094596	0.666365933	0.978791948
0.166505651	0.334292926	0.320874814

Interpolating coordinate: 0.417 (-829.708 eV)

0.180980611	0.013914414	0.082982385
0.332751256	0.319674846	0.083664117
0.488726527	0.166307227	0.082469835
0.680912495	0.013151656	0.084386072
0.835425365	0.321571926	0.085757034
0.985495740	0.171355347	0.083049028
0.179772659	0.513991613	0.083828689
0.333314242	0.818883600	0.084115967
0.483806572	0.662774085	0.086004783
0.680327007	0.510907052	0.083054177
0.826782222	0.811910998	0.082853622
0.986868852	0.668395198	0.083238307
0.155409669	0.176545261	0.260586467
0.015972746	0.343495702	0.258844038
0.347613067	0.000320757	0.250956050
0.655861798	0.153451271	0.250345368
0.503218612	0.351621289	0.250199907
0.845674638	-0.001560831	0.250014103
0.152087786	0.652807822	0.249649477
0.001324035	0.848020932	0.252091095
0.325488365	0.483868769	0.258730952
0.648981316	0.651488330	0.249584358
0.497821107	0.844040700	0.250802900
0.849912532	0.498997333	0.249217924
0.021756710	0.191436146	0.411200661
0.309450834	0.332648579	0.411039580
0.168197763	0.477781165	0.410086762
0.512534331	0.180960667	0.415810725
0.819648173	0.334224452	0.416335839
0.666219845	0.486919355	0.416431755
0.014093628	0.678867867	0.417078931
0.319876756	0.832094753	0.416552808
0.166239141	0.986241402	0.416304880
0.514271450	0.680226612	0.416560117
0.820981673	0.835243050	0.416424721
0.667602686	0.987717844	0.416479830
0.484126971	0.320235337	0.581049232
0.179505181	0.165855939	0.582519607

0.333463603	0.013899847	0.582280974
0.986213898	0.320548157	0.582552635
0.680288041	0.166950957	0.582340134
0.835862067	0.016017757	0.581486673
0.486418203	0.819647329	0.582375602
0.180026061	0.664069556	0.581226514
0.333968813	0.513674953	0.582413628
0.986816024	0.819546804	0.583138592
0.680792957	0.667560573	0.583060439
0.832581445	0.513451805	0.583095262
0.346575148	0.346762039	0.749325183
0.153329131	0.000189926	0.749614891
-0.000030980	0.153129937	0.749615788
0.846819655	0.346870730	0.749450756
0.653088742	-0.000488631	0.749416587
0.500350422	0.153259215	0.749165794
0.346817591	0.846945254	0.749169221
0.153179735	0.499885278	0.749314641
0.000503548	0.653340161	0.749352835
0.846766689	0.847069245	0.749618696
0.652759490	0.499495144	0.749388936
0.499875098	0.653091017	0.749501391
0.319638802	0.486797477	0.916612072
0.166972032	0.180519006	0.916891045
0.013598725	0.333533087	0.916174130
0.820137464	0.486165409	0.916419255
0.667703835	0.179954252	0.916483931
0.513631892	0.332921282	0.916436892
0.320086408	0.986373302	0.916420528
0.166818841	0.680274804	0.916536425
0.013350796	0.833086593	0.916251662
0.819518009	0.985377822	0.917087159
0.665185017	0.679170119	0.916188311
0.513104133	0.832884375	0.917219683
0.166247672	0.333359419	0.021065934
0.667937964	0.331460657	0.020915003
0.168242651	0.835354529	0.020850364
0.664463360	0.831380173	0.022192857
0.000014425	-0.001104589	0.144101431
0.500215404	0.001014078	0.146073910
0.001292833	0.504318490	0.144652811
0.502200530	0.495501109	0.144667690
0.327658236	0.166066197	0.189711440
0.839423428	0.167905636	0.188639489

0.331184981	0.662060235	0.189061139
0.834587589	0.671024248	0.187200514
0.666531995	0.333298217	0.311420986
0.167919997	0.833762365	0.312879913
0.666348243	0.833787101	0.312594033
0.001060629	0.001913613	0.351004576
0.500051603	0.000274880	0.353222707
-0.000633692	0.499666519	0.352512025
0.499750312	0.499819171	0.352560344
0.331543756	0.165652847	0.477880392
0.833551171	0.168617900	0.478297920
0.334917845	0.666262300	0.478305641
0.833722599	0.667500406	0.478843128
0.166364796	0.333044705	0.523683024
0.665816785	0.333931632	0.519918352
0.166637193	0.832376900	0.520308891
0.668088774	0.834594642	0.520144341
-0.000318302	-0.000765611	0.646329010
0.500092686	0.000058414	0.645531309
-0.000626667	0.500312889	0.646061455
0.500810366	0.500682499	0.646022107
0.333487357	0.166670351	0.686968862
0.833171255	0.166580255	0.687177036
0.333365638	0.666696766	0.687028935
0.833256792	0.666627835	0.687193455
0.166513171	0.333280968	0.813044973
0.666689786	0.333252081	0.813000616
0.166877179	0.833547113	0.812822842
0.666541706	0.832845344	0.813252807
0.000344990	0.000402124	0.854594451
0.500444027	-0.000046431	0.854175998
0.000275043	0.500070907	0.853915952
0.498967770	0.498842776	0.854013700
0.334195753	0.166706707	0.981146052
0.834343942	0.165934686	0.980196615
0.332670266	0.666468311	0.980154657
0.832276787	0.666397953	0.978773647
0.166233787	0.334227199	0.320816194

Interpolating coordinate: 0.420 (-829.693 eV)

0.180946378	0.013895249	0.082965689
0.332753877	0.319674279	0.083659614
0.488737037	0.166298479	0.082453884
0.680916290	0.013153099	0.084386627

0.835432667	0.321566366	0.085755950
0.985505998	0.171332016	0.083053605
0.179773725	0.513986015	0.083828047
0.333312257	0.818879116	0.084113517
0.483812527	0.662774086	0.086006752
0.680338630	0.510922141	0.083054027
0.826819678	0.811954101	0.082860165
0.986867268	0.668390336	0.083236922
0.155365537	0.176533211	0.260585671
0.015962285	0.343498817	0.258843354
0.347617420	0.000303765	0.250953861
0.655859190	0.153454121	0.250345037
0.503238263	0.351651017	0.250204544
0.845667850	-0.001561126	0.250014452
0.152087542	0.652808907	0.249647804
0.001333448	0.848048865	0.252074657
0.325480393	0.483863438	0.258728897
0.648990985	0.651499169	0.249583280
0.497823197	0.844037087	0.250801980
0.849914231	0.499003852	0.249218769
0.021746948	0.191438018	0.411206667
0.309441549	0.332641584	0.411035476
0.168194447	0.477780968	0.410085746
0.512532614	0.180961048	0.415809584
0.819647577	0.334228009	0.416337727
0.666219218	0.486921448	0.416435938
0.014091474	0.678874067	0.417074097
0.319873476	0.832092724	0.416552531
0.166238537	0.986242970	0.416301829
0.514269818	0.680225677	0.416559722
0.820981377	0.835243350	0.416425639
0.667600804	0.987717862	0.416480380
0.484125541	0.320235754	0.581049043
0.179504115	0.165855861	0.582518978
0.333463112	0.013899903	0.582279886
0.986212912	0.320548352	0.582555109
0.680286629	0.166952164	0.582341368
0.835859684	0.016016897	0.581488223
0.486416858	0.819646170	0.582375872
0.180024988	0.664069245	0.581225499
0.333967961	0.513674021	0.582413397
0.986817119	0.819547809	0.583138157
0.680792753	0.667561782	0.583061872
0.832582093	0.513453279	0.583095899

0.346577315	0.346762785	0.749325154
0.153329363	0.000189663	0.749613287
-0.000030426	0.153129750	0.749616171
0.846820792	0.346871017	0.749451387
0.653088373	-0.000489618	0.749417143
0.500350296	0.153258923	0.749165599
0.346818905	0.846944701	0.749168761
0.153180851	0.499884317	0.749315392
0.000504003	0.653338654	0.749351999
0.846766674	0.847069351	0.749619044
0.652760663	0.499496676	0.749390235
0.499876208	0.653091512	0.749503415
0.319640886	0.486797505	0.916611829
0.166976476	0.180519816	0.916888769
0.013599096	0.333529063	0.916177117
0.820140467	0.486166780	0.916419199
0.667711347	0.179955511	0.916479950
0.513636381	0.332922682	0.916437247
0.320085253	0.986370333	0.916418042
0.166820079	0.680271762	0.916535232
0.013348023	0.833080350	0.916245405
0.819520729	0.985378490	0.917087733
0.665189620	0.679172909	0.916194190
0.513108135	0.832885610	0.917221922
0.166255755	0.333358132	0.021063368
0.667942275	0.331462679	0.020913980
0.168239853	0.835347049	0.020845038
0.664465677	0.831380974	0.022196580
0.000030580	-0.001085924	0.144107981
0.500209037	0.001014461	0.146070890
0.001298621	0.504317063	0.144653766
0.502195024	0.495487713	0.144671686
0.327647060	0.166049701	0.189713838
0.839410242	0.167902521	0.188643225
0.331188713	0.662060731	0.189061791
0.834580827	0.671011663	0.187201898
0.666526872	0.333301795	0.311421927
0.167921114	0.833766096	0.312875425
0.666345455	0.833784461	0.312594889
0.001056777	0.001921681	0.351013457
0.500048566	0.000272672	0.353220826
-0.000635996	0.499669215	0.352513336
0.499747634	0.499814514	0.352559619
0.331542852	0.165653916	0.477878141

0.833544712	0.168618769	0.478300405
0.334916906	0.666261090	0.478304659
0.833722091	0.667501790	0.478844674
0.166361484	0.333043878	0.523682810
0.665816106	0.333933711	0.519918322
0.166637928	0.832377329	0.520306840
0.668087214	0.834594617	0.520144195
-0.000318799	-0.000765690	0.646328336
0.500091670	0.000057823	0.645530692
-0.000626520	0.500313646	0.646061828
0.500810135	0.500683034	0.646022534
0.333487677	0.166670723	0.686967566
0.833171348	0.166579972	0.687177963
0.333366240	0.666695723	0.687028834
0.833257456	0.666628475	0.687193625
0.166515679	0.333279735	0.813044467
0.666689872	0.333251425	0.812999743
0.166877838	0.833546469	0.812820197
0.666543443	0.832846602	0.813254176
0.000347860	0.000402900	0.854593231
0.500444535	-0.000047049	0.854175902
0.000276684	0.500067734	0.853915898
0.498971923	0.498844417	0.854015418
0.334200365	0.166704414	0.981150755
0.834341874	0.165931351	0.980196430
0.332672670	0.666467847	0.980155688
0.832284075	0.666399234	0.978772915
0.166222912	0.334224570	0.320813849

Interpolating coordinate: 0.423 (-829.696 eV)

0.180912145	0.013876083	0.082948992
0.332756499	0.319673712	0.083655112
0.488747548	0.166289732	0.082437933
0.680920085	0.013154542	0.084387183
0.835439968	0.321560806	0.085754865
0.985516257	0.171308685	0.083058182
0.179774792	0.513980417	0.083827404
0.333310272	0.818874633	0.084111067
0.483818482	0.662774087	0.086008721
0.680350253	0.510937230	0.083053876
0.826857135	0.811997204	0.082866708
0.986865684	0.668385474	0.083235537
0.155321404	0.176521160	0.260584875
0.015951824	0.343501933	0.258842670

0.347621773	0.000286773	0.250951671
0.655856582	0.153456970	0.250344706
0.503257913	0.351680745	0.250209180
0.845661062	-0.001561421	0.250014801
0.152087297	0.652809992	0.249646132
0.001342861	0.848076798	0.252058219
0.325472422	0.483858107	0.258726842
0.649000654	0.651510009	0.249582201
0.497825287	0.844033473	0.250801059
0.849915930	0.499010371	0.249219614
0.021737186	0.191439890	0.411212673
0.309432263	0.332634589	0.411031371
0.168191130	0.477780770	0.410084729
0.512530897	0.180961429	0.415808442
0.819646980	0.334231566	0.416339615
0.666218591	0.486923541	0.416440120
0.014089320	0.678880267	0.417069263
0.319870196	0.832090695	0.416552254
0.166237933	0.986244537	0.416298777
0.514268187	0.680224742	0.416559328
0.820981080	0.835243649	0.416426558
0.667598922	0.987717880	0.416480930
0.484124111	0.320236172	0.581048854
0.179503050	0.165855783	0.582518349
0.333462622	0.013899958	0.582278799
0.986211926	0.320548547	0.582557584
0.680285217	0.166953371	0.582342602
0.835857300	0.016016037	0.581489773
0.486415513	0.819645011	0.582376141
0.180023915	0.664068934	0.581224484
0.333967109	0.513673088	0.582413166
0.986818214	0.819548814	0.583137722
0.680792549	0.667562992	0.583063305
0.832582741	0.513454753	0.583096536
0.346579482	0.346763531	0.749325125
0.153329595	0.000189401	0.749611682
-0.000029872	0.153129562	0.749616553
0.846821929	0.346871303	0.749452018
0.653088003	-0.000490604	0.749417699
0.500350171	0.153258631	0.749165404
0.346820220	0.846944148	0.749168301
0.153181968	0.499883356	0.749316143
0.000504457	0.653337147	0.749351164
0.846766660	0.847069458	0.749619392

0.652761835	0.499498208	0.749391534
0.499877318	0.653092007	0.749505439
0.319642969	0.486797533	0.916611586
0.166980920	0.180520626	0.916886493
0.013599467	0.333525039	0.916180105
0.820143470	0.486168150	0.916419143
0.667718859	0.179956770	0.916475968
0.513640869	0.332924082	0.916437603
0.320084098	0.986367363	0.916415556
0.166821318	0.680268719	0.916534039
0.013345250	0.833074108	0.916239148
0.819523449	0.985379158	0.917088308
0.665194222	0.679175699	0.916200068
0.513112137	0.832886845	0.917224162
0.166263839	0.333356844	0.021060802
0.667946585	0.331464701	0.020912958
0.168237055	0.835339568	0.020839711
0.664467994	0.831381775	0.022200303
0.000046736	-0.001067260	0.144114530
0.500202671	0.001014844	0.146067870
0.001304410	0.504315636	0.144654722
0.502189519	0.495474317	0.144675682
0.327635885	0.166033205	0.189716237
0.839397057	0.167899406	0.188646961
0.331192444	0.662061227	0.189062442
0.834574065	0.670999077	0.187203283
0.666521749	0.333305373	0.311422867
0.167922231	0.833769827	0.312870936
0.666342668	0.833781820	0.312595744
0.001052926	0.001929749	0.351022339
0.500045528	0.000270464	0.353218946
-0.000638300	0.499671911	0.352514647
0.499744956	0.499809858	0.352558895
0.331541948	0.165654985	0.477875890
0.833538253	0.168619638	0.478302890
0.334915968	0.666259880	0.478303677
0.833721583	0.667503173	0.478846220
0.166358172	0.333043051	0.523682596
0.665815427	0.333935791	0.519918291
0.166638663	0.832377759	0.520304790
0.668085654	0.834594593	0.520144048
-0.000319296	-0.000765769	0.646327662
0.500090654	0.000057233	0.645530075
-0.000626372	0.500314403	0.646062202

0.500809903	0.500683569	0.646022961
0.333487997	0.166671095	0.686966269
0.833171441	0.166579689	0.687178889
0.333366842	0.666694680	0.687028733
0.833258120	0.666629116	0.687193795
0.166518187	0.333278501	0.813043961
0.666689958	0.333250769	0.812998870
0.166878497	0.833545826	0.812817552
0.666545180	0.832847861	0.813255545
0.000350731	0.000403676	0.854592011
0.500445044	-0.000047668	0.854175807
0.000278325	0.500064561	0.853915844
0.498976076	0.498846058	0.854017136
0.334204977	0.166702121	0.981155458
0.834339806	0.165928016	0.980196244
0.332675073	0.666467383	0.980156720
0.832291362	0.666400515	0.978772183
0.166212038	0.334221941	0.320811504

Interpolating coordinate: 0.427 (-829.696 eV)

0.180877913	0.013856918	0.082932296
0.332759120	0.319673145	0.083650609
0.488758058	0.166280984	0.082421982
0.680923879	0.013155984	0.084387738
0.835447270	0.321555245	0.085753781
0.985526515	0.171285353	0.083062759
0.179775858	0.513974819	0.083826762
0.333308288	0.818870149	0.084108617
0.483824438	0.662774089	0.086010690
0.680361875	0.510952320	0.083053726
0.826894591	0.812040307	0.082873251
0.986864101	0.668380613	0.083234152
0.155277272	0.176509110	0.260584078
0.015941362	0.343505048	0.258841985
0.347626126	0.000269782	0.250949482
0.655853975	0.153459820	0.250344375
0.503277564	0.351710474	0.250213817
0.845654274	-0.001561715	0.250015149
0.152087053	0.652811077	0.249644459
0.001352275	0.848104732	0.252041781
0.325464450	0.483852777	0.258724786
0.649010323	0.651520848	0.249581123
0.497827378	0.844029860	0.250800139
0.849917628	0.499016890	0.249220458

0.021727423	0.191441761	0.411218679
0.309422978	0.332627593	0.411027267
0.168187814	0.477780573	0.410083713
0.512529181	0.180961810	0.415807301
0.819646384	0.334235122	0.416341503
0.666217964	0.486925633	0.416444303
0.014087167	0.678886468	0.417064430
0.319866915	0.832088665	0.416551977
0.166237330	0.986246105	0.416295726
0.514266555	0.680223806	0.416558933
0.820980784	0.835243949	0.416427476
0.667597041	0.987717899	0.416481481
0.484122680	0.320236589	0.581048665
0.179501984	0.165855705	0.582517720
0.333462131	0.013900014	0.582277711
0.986210940	0.320548741	0.582560058
0.680283806	0.166954577	0.582343837
0.835854917	0.016015178	0.581491322
0.486414169	0.819643851	0.582376411
0.180022843	0.664068624	0.581223469
0.333966256	0.513672156	0.582412934
0.986819308	0.819549818	0.583137288
0.680792344	0.667564201	0.583064739
0.832583390	0.513456227	0.583097174
0.346581649	0.346764278	0.749325096
0.153329827	0.000189138	0.749610078
-0.000029318	0.153129375	0.749616936
0.846823066	0.346871590	0.749452648
0.653087634	-0.000491591	0.749418255
0.500350045	0.153258339	0.749165209
0.346821534	0.846943595	0.749167841
0.153183084	0.499882394	0.749316893
0.000504912	0.653335641	0.749350328
0.846766645	0.847069564	0.749619741
0.652763008	0.499499739	0.749392832
0.499878429	0.653092502	0.749507462
0.319645053	0.486797562	0.916611344
0.166985364	0.180521435	0.916884218
0.013599838	0.333521016	0.916183092
0.820146474	0.486169521	0.916419087
0.667726370	0.179958030	0.916471987
0.513645358	0.332925481	0.916437958
0.320082942	0.986364394	0.916413070
0.166822556	0.680265677	0.916532845

0.013342478	0.833067865	0.916232890
0.819526170	0.985379827	0.917088882
0.665198825	0.679178489	0.916205947
0.513116140	0.832888081	0.917226401
0.166271922	0.333355557	0.021058235
0.667950896	0.331466722	0.020911935
0.168234256	0.835332088	0.020834385
0.664470312	0.831382577	0.022204026
0.000062891	-0.001048595	0.144121080
0.500196304	0.001015227	0.146064851
0.001310198	0.504314209	0.144655677
0.502184013	0.495460921	0.144679678
0.327624709	0.166016708	0.189718635
0.839383871	0.167896292	0.188650698
0.331196176	0.662061723	0.189063094
0.834567303	0.670986492	0.187204667
0.666516627	0.333308950	0.311423808
0.167923349	0.833773557	0.312866448
0.666339880	0.833779180	0.312596600
0.001049074	0.001937817	0.351031220
0.500042491	0.000268256	0.353217065
-0.000640605	0.499674607	0.352515958
0.499742279	0.499805201	0.352558170
0.331541043	0.165656053	0.477873639
0.833531795	0.168620506	0.478305375
0.334915029	0.666258670	0.478302695
0.833721076	0.667504557	0.478847766
0.166354859	0.333042225	0.523682381
0.665814749	0.333937870	0.519918261
0.166639399	0.832378188	0.520302739
0.668084094	0.834594568	0.520143902
-0.000319792	-0.000765848	0.646326987
0.500089638	0.000056642	0.645529459
-0.000626225	0.500315160	0.646062575
0.500809672	0.500684104	0.646023387
0.333488318	0.166671468	0.686964973
0.833171534	0.166579405	0.687179816
0.333367443	0.666693636	0.687028632
0.833258784	0.666629756	0.687193964
0.166520694	0.333277268	0.813043454
0.666690044	0.333250112	0.812997997
0.166879157	0.833545182	0.812814907
0.666546916	0.832849119	0.813256913
0.000353601	0.000404452	0.854590790

0.500445552	-0.000048286	0.854175711
0.000279967	0.500061388	0.853915789
0.498980230	0.498847698	0.854018853
0.334209590	0.166699828	0.981160160
0.834337739	0.165924682	0.980196059
0.332677477	0.666466920	0.980157751
0.832298650	0.666401795	0.978771451
0.166201163	0.334219312	0.320809160

Interpolating coordinate: 0.430 (-829.697 eV)

0.180843680	0.013837752	0.082915599
0.332761742	0.319672578	0.083646107
0.488768569	0.166272237	0.082406031
0.680927674	0.013157427	0.084388294
0.835454571	0.321549685	0.085752696
0.985536774	0.171262022	0.083067336
0.179776925	0.513969221	0.083826119
0.333306303	0.818865666	0.084106167
0.483830393	0.662774090	0.086012659
0.680373498	0.510967409	0.083053575
0.826932048	0.812083410	0.082879794
0.986862517	0.668375751	0.083232767
0.155233139	0.176497059	0.260583282
0.015930901	0.343508164	0.258841301
0.347630479	0.000252790	0.250947292
0.655851367	0.153462669	0.250344044
0.503297214	0.351740202	0.250218453
0.845647486	-0.001562010	0.250015498
0.152086808	0.652812162	0.249642787
0.001361688	0.848132665	0.252025343
0.325456479	0.483847446	0.258722731
0.649019992	0.651531688	0.249580044
0.497829468	0.844026246	0.250799218
0.849919327	0.499023409	0.249221303
0.021717661	0.191443633	0.411224685
0.309413692	0.332620598	0.411023162
0.168184497	0.477780375	0.410082696
0.512527464	0.180962191	0.415806159
0.819645787	0.334238679	0.416343391
0.666217337	0.486927726	0.416448485
0.014085013	0.678892668	0.417059596
0.319863635	0.832086636	0.416551700
0.166236726	0.986247672	0.416292674
0.514264924	0.680222871	0.416558539

0.820980487	0.835244248	0.416428395
0.667595159	0.987717917	0.416482031
0.484121250	0.320237007	0.581048476
0.179500919	0.165855627	0.582517091
0.333461641	0.013900069	0.582276624
0.986209954	0.320548936	0.582562533
0.680282394	0.166955784	0.582345071
0.835852533	0.016014318	0.581492872
0.486412824	0.819642692	0.582376680
0.180021770	0.664068313	0.581222454
0.333965404	0.513671223	0.582412703
0.986820403	0.819550823	0.583136853
0.680792140	0.667565411	0.583066172
0.832584038	0.513457701	0.583097811
0.346583816	0.346765024	0.749325067
0.153330059	0.000188876	0.749608473
-0.000028764	0.153129187	0.749617318
0.846824203	0.346871876	0.749453279
0.653087264	-0.000492577	0.749418811
0.500349920	0.153258047	0.749165014
0.346822849	0.846943042	0.749167381
0.153184201	0.499881433	0.749317644
0.000505366	0.653334134	0.749349493
0.846766631	0.847069671	0.749620089
0.652764180	0.499501271	0.749394131
0.499879539	0.653092997	0.749509486
0.319647136	0.486797590	0.916611101
0.166989808	0.180522245	0.916881942
0.013600209	0.333516992	0.916186080
0.820149477	0.486170891	0.916419031
0.667733882	0.179959289	0.916468005
0.513649846	0.332926881	0.916438314
0.320081787	0.986361424	0.916410584
0.166823795	0.680262634	0.916531652
0.013339705	0.833061623	0.916226633
0.819528890	0.985380495	0.917089457
0.665203427	0.679181279	0.916211825
0.513120142	0.832889316	0.917228641
0.166280006	0.333354269	0.021055669
0.667955206	0.331468744	0.020910913
0.168231458	0.835324607	0.020829058
0.664472629	0.831383378	0.022207749
0.000079047	-0.001029931	0.144127629
0.500189938	0.001015610	0.146061831

0.001315987	0.504312782	0.144656633
0.502178508	0.495447525	0.144683674
0.327613534	0.166000212	0.189721034
0.839370686	0.167893177	0.188654434
0.331199907	0.662062219	0.189063745
0.834560541	0.670973906	0.187206052
0.666511504	0.333312528	0.311424748
0.167924466	0.833777288	0.312861959
0.666337093	0.833776539	0.312597455
0.001045223	0.001945885	0.351040102
0.500039453	0.000266048	0.353215185
-0.000642909	0.499677303	0.352517269
0.499739601	0.499800545	0.352557446
0.331540139	0.165657122	0.477871388
0.833525336	0.168621375	0.478307860
0.334914091	0.666257460	0.478301713
0.833720568	0.667505940	0.478849312
0.166351547	0.333041398	0.523682167
0.665814070	0.333939950	0.519918230
0.166640134	0.832378618	0.520300689
0.668082534	0.834594544	0.520143755
-0.000320289	-0.000765927	0.646326313
0.500088622	0.000056052	0.645528842
-0.000626077	0.500315917	0.646062949
0.500809440	0.500684639	0.646023814
0.333488638	0.166671840	0.686963676
0.833171627	0.166579122	0.687180742
0.333368045	0.666692593	0.687028531
0.833259448	0.666630397	0.687194134
0.166523202	0.333276034	0.813042948
0.666690130	0.333249456	0.812997124
0.166879816	0.833544539	0.812812262
0.666548653	0.832850378	0.813258282
0.000356472	0.000405228	0.854589570
0.500446061	-0.000048905	0.854175616
0.000281608	0.500058215	0.853915735
0.498984383	0.498849339	0.854020571
0.334214202	0.166697535	0.981164863
0.834335671	0.165921347	0.980195873
0.332679880	0.666466456	0.980158783
0.832305937	0.666403076	0.978770719
0.166190289	0.334216683	0.320806815

Interpolating coordinate: 0.433 (-829.699 eV)

0.180809447	0.013818587	0.082898903
0.332764363	0.319672011	0.083641604
0.488779079	0.166263489	0.082390080
0.680931469	0.013158870	0.084388849
0.835461873	0.321544125	0.085751612
0.985547032	0.171238691	0.083071913
0.179777991	0.513963623	0.083825477
0.333304318	0.818861182	0.084103717
0.483836348	0.662774091	0.086014628
0.680385121	0.510982498	0.083053425
0.826969504	0.812126513	0.082886337
0.986860933	0.668370889	0.083231382
0.155189007	0.176485009	0.260582486
0.015920440	0.343511279	0.258840617
0.347634832	0.000235798	0.250945103
0.655848759	0.153465519	0.250343713
0.503316865	0.351769930	0.250223090
0.845640698	-0.001562305	0.250015847
0.152086564	0.652813247	0.249641114
0.001371101	0.848160598	0.252008905
0.325448507	0.483842115	0.258720676
0.649029661	0.651542527	0.249578966
0.497831558	0.844022633	0.250798298
0.849921026	0.499029928	0.249222148
0.021707899	0.191445505	0.411230691
0.309404407	0.332613603	0.411019058
0.168181181	0.477780178	0.410081680
0.512525747	0.180962572	0.415805018
0.819645191	0.334242236	0.416345279
0.666216710	0.486929819	0.416452668
0.014082859	0.678898868	0.417054762
0.319860355	0.832084607	0.416551423
0.166236122	0.986249240	0.416289623
0.514263292	0.680221936	0.416558144
0.820980191	0.835244548	0.416429313
0.667593277	0.987717935	0.416482581
0.484119820	0.320237424	0.581048287
0.179499853	0.165855549	0.582516462
0.333461150	0.013900125	0.582275536
0.986208968	0.320549131	0.582565007
0.680280982	0.166956991	0.582346305
0.835850150	0.016013458	0.581494422
0.486411479	0.819641533	0.582376950
0.180020697	0.664068002	0.581221439

0.333964552	0.513670291	0.582412472
0.986821498	0.819551828	0.583136418
0.680791936	0.667566620	0.583067605
0.832584686	0.513459175	0.583098448
0.346585983	0.346765770	0.749325038
0.153330291	0.000188613	0.749606869
-0.000028210	0.153129000	0.749617701
0.846825340	0.346872163	0.749453910
0.653086895	-0.000493564	0.749419367
0.500349794	0.153257755	0.749164819
0.346824163	0.846942489	0.749166921
0.153185317	0.499880472	0.749318395
0.000505821	0.653332627	0.749348657
0.846766616	0.847069777	0.749620437
0.652765353	0.499502803	0.749395430
0.499880649	0.653093492	0.749511510
0.319649220	0.486797618	0.916610858
0.166994252	0.180523055	0.916879666
0.013600580	0.333512968	0.916189067
0.820152480	0.486172262	0.916418975
0.667741394	0.179960548	0.916464024
0.513654335	0.332928281	0.916438669
0.320080632	0.986358455	0.916408098
0.166825033	0.680259592	0.916530459
0.013336932	0.833055380	0.916220376
0.819531610	0.985381163	0.917090031
0.665208030	0.679184069	0.916217704
0.513124144	0.832890551	0.917230880
0.166288089	0.333352982	0.021053103
0.667959517	0.331470766	0.020909890
0.168228660	0.835317127	0.020823732
0.664474946	0.831384179	0.022211472
0.000095202	-0.001011266	0.144134179
0.500183571	0.001015993	0.146058811
0.001321775	0.504311355	0.144657588
0.502173002	0.495434129	0.144687670
0.327602358	0.165983716	0.189723432
0.839357500	0.167890062	0.188658170
0.331203639	0.662062715	0.189064397
0.834553779	0.670961321	0.187207436
0.666506381	0.333316106	0.311425689
0.167925583	0.833781019	0.312857471
0.666334305	0.833773899	0.312598311
0.001041371	0.001953953	0.351048983

0.500036416	0.000263840	0.353213304
-0.000645213	0.499679999	0.352518580
0.499736923	0.499795888	0.352556721
0.331539235	0.165658191	0.477869137
0.833518877	0.168622244	0.478310345
0.334913152	0.666256250	0.478300731
0.833720060	0.667507324	0.478850858
0.166348235	0.333040571	0.523681953
0.665813391	0.333942029	0.519918200
0.166640869	0.832379047	0.520298638
0.668080974	0.834594519	0.520143609
-0.000320786	-0.000766006	0.646325639
0.500087606	0.000055461	0.645528225
-0.000625930	0.500316674	0.646063322
0.500809209	0.500685174	0.646024241
0.333488958	0.166672212	0.686962380
0.833171720	0.166578839	0.687181669
0.333368647	0.666691550	0.687028430
0.833260112	0.666631037	0.687194304
0.166525710	0.333274801	0.813042442
0.666690216	0.333248800	0.812996251
0.166880475	0.833543895	0.812809617
0.666550390	0.832851636	0.813259651
0.000359342	0.000406004	0.854588350
0.500446569	-0.000049523	0.854175520
0.000283249	0.500055042	0.853915681
0.498988536	0.498850980	0.854022289
0.334218814	0.166695242	0.981169566
0.834333603	0.165918012	0.980195688
0.332682284	0.666465992	0.980159814
0.832313225	0.666404357	0.978769987
0.166179414	0.334214054	0.320804470

Interpolating coordinate: 0.450 (-829.709 eV)

0.180638283	0.013722760	0.082815422
0.332777470	0.319669176	0.083619091
0.488831632	0.166219752	0.082310325
0.680950444	0.013166083	0.084391627
0.835498381	0.321516325	0.085746190
0.985598325	0.171122035	0.083094798
0.179783323	0.513935632	0.083822264
0.333294393	0.818838764	0.084091467
0.483866124	0.662774097	0.086024473
0.680443236	0.511057945	0.083052672

0.827156787	0.812342029	0.082919052
0.986853014	0.668346581	0.083224457
0.154968344	0.176424757	0.260578505
0.015868134	0.343526855	0.258837196
0.347656597	0.000150839	0.250934156
0.655835720	0.153479767	0.250342058
0.503415118	0.351918570	0.250246274
0.845606757	-0.001563778	0.250017591
0.152085342	0.652818673	0.249632752
0.001418168	0.848300263	0.251926714
0.325408648	0.483815460	0.258710401
0.649078006	0.651596725	0.249573574
0.497842009	0.844004566	0.250793696
0.849929520	0.499062522	0.249226371
0.021659088	0.191454864	0.411260721
0.309357979	0.332578628	0.410998535
0.168164599	0.477779191	0.410076597
0.512517163	0.180964477	0.415799311
0.819642210	0.334260021	0.416354718
0.666213576	0.486940283	0.416473581
0.014072090	0.678929869	0.417030593
0.319843955	0.832074462	0.416550038
0.166233103	0.986257077	0.416274366
0.514255135	0.680217260	0.416556171
0.820978708	0.835246046	0.416433906
0.667583867	0.987718026	0.416485332
0.484112670	0.320239511	0.581047342
0.179494526	0.165855160	0.582513316
0.333458697	0.013900402	0.582270098
0.986204038	0.320550105	0.582577378
0.680273923	0.166963025	0.582352476
0.835838233	0.016009160	0.581502171
0.486404754	0.819635737	0.582378298
0.180015333	0.664066448	0.581216364
0.333960290	0.513665629	0.582411315
0.986826973	0.819556853	0.583134244
0.680790915	0.667572668	0.583074771
0.832587927	0.513466544	0.583101633
0.346596818	0.346769501	0.749324894
0.153331452	0.000187301	0.749598846
-0.000025441	0.153128063	0.749619614
0.846831025	0.346873597	0.749457063
0.653085048	-0.000498497	0.749422146
0.500349165	0.153256295	0.749163845

0.346830736	0.846939724	0.749164621
0.153190900	0.499875666	0.749322149
0.000508095	0.653325093	0.749344480
0.846766543	0.847070308	0.749622178
0.652771215	0.499510463	0.749401925
0.499886200	0.653095967	0.749521628
0.319659638	0.486797760	0.916609643
0.167016471	0.180527103	0.916868287
0.013602435	0.333492848	0.916204003
0.820167496	0.486179115	0.916418695
0.667778954	0.179966843	0.916444117
0.513676778	0.332935281	0.916440446
0.320074856	0.986343609	0.916395667
0.166831225	0.680244380	0.916524493
0.013323067	0.833024167	0.916189090
0.819545211	0.985384503	0.917092903
0.665231043	0.679198018	0.916247097
0.513144156	0.832896728	0.917242076
0.166328507	0.333346544	0.021040272
0.667981070	0.331480875	0.020904777
0.168214670	0.835279725	0.020797100
0.664486531	0.831388184	0.022230086
0.000175978	-0.000917942	0.144166927
0.500151738	0.001017908	0.146043711
0.001350717	0.504304219	0.144662365
0.502145474	0.495367149	0.144707650
0.327546481	0.165901235	0.189735424
0.839291572	0.167874488	0.188676851
0.331222297	0.662065195	0.189067655
0.834519969	0.670898394	0.187214359
0.666480767	0.333333995	0.311430393
0.167931169	0.833799672	0.312835029
0.666320367	0.833760697	0.312602590
0.001022113	0.001994293	0.351093390
0.500021228	0.000252800	0.353203900
-0.000656734	0.499693479	0.352525135
0.499723534	0.499772605	0.352553098
0.331534713	0.165663536	0.477857883
0.833486583	0.168626587	0.478322771
0.334908460	0.666250200	0.478295821
0.833717521	0.667514242	0.478858588
0.166331674	0.333036437	0.523680882
0.665809996	0.333952426	0.519918048
0.166644545	0.832381193	0.520288386

0.668073175	0.834594397	0.520142877
-0.000323270	-0.000766401	0.646322268
0.500082527	0.000052509	0.645525142
-0.000625193	0.500320459	0.646065189
0.500808052	0.500687848	0.646026375
0.333490558	0.166674072	0.686955899
0.833172185	0.166577424	0.687186303
0.333371655	0.666686334	0.687027924
0.833263432	0.666634239	0.687195154
0.166538249	0.333268634	0.813039912
0.666690646	0.333245519	0.812991886
0.166883772	0.833540677	0.812796393
0.666559074	0.832857927	0.813266495
0.000373693	0.000409884	0.854582249
0.500449110	-0.000052615	0.854175042
0.000291455	0.500039177	0.853915410
0.499009301	0.498859185	0.854030878
0.334241875	0.166683778	0.981193080
0.834323264	0.165901337	0.980194761
0.332694303	0.666463672	0.980164970
0.832349663	0.666410761	0.978766327
0.166125041	0.334200908	0.320792746

Interpolating coordinate: 0.467 (-829.718 eV)

0.180467119	0.013626934	0.082731940
0.332790577	0.319666340	0.083596579
0.488884184	0.166176014	0.082230571
0.680969418	0.013173297	0.084394404
0.835534890	0.321488524	0.085740768
0.985649617	0.171005380	0.083117682
0.179788655	0.513907642	0.083819052
0.333284469	0.818816347	0.084079217
0.483895901	0.662774103	0.086034317
0.680501350	0.511133391	0.083051920
0.827344069	0.812557544	0.082951766
0.986845096	0.668322272	0.083217532
0.154747682	0.176364506	0.260574525
0.015815829	0.343542432	0.258833775
0.347678363	0.000065881	0.250923210
0.655822681	0.153494016	0.250340404
0.503513370	0.352067211	0.250269457
0.845572817	-0.001565252	0.250019335
0.152084121	0.652824098	0.249624389
0.001465234	0.848439929	0.251844524

0.325368790	0.483788806	0.258700125
0.649126351	0.651650922	0.249568183
0.497852460	0.843986498	0.250789095
0.849938015	0.499095117	0.249230595
0.021610277	0.191464224	0.411290751
0.309311552	0.332543652	0.410978013
0.168148018	0.477778203	0.410071515
0.512508579	0.180966381	0.415793603
0.819639228	0.334277805	0.416364158
0.666210441	0.486950746	0.416494495
0.014061321	0.678960869	0.417006424
0.319827554	0.832064316	0.416548653
0.166230084	0.986264915	0.416259110
0.514246977	0.680212584	0.416554197
0.820977226	0.835247545	0.416438498
0.667574458	0.987718118	0.416488083
0.484105519	0.320241597	0.581046398
0.179489198	0.165854770	0.582510171
0.333456244	0.013900680	0.582264659
0.986199108	0.320551079	0.582589750
0.680266865	0.166969058	0.582358647
0.835826316	0.016004861	0.581509920
0.486398030	0.819629940	0.582379647
0.180009969	0.664064893	0.581211290
0.333956029	0.513660966	0.582410159
0.986832447	0.819561877	0.583132071
0.680789893	0.667578715	0.583081937
0.832591168	0.513473914	0.583104819
0.346607654	0.346773231	0.749324749
0.153332612	0.000185988	0.749590824
-0.000022671	0.153127126	0.749621526
0.846836711	0.346875030	0.749460217
0.653083202	-0.000503429	0.749424926
0.500348537	0.153254835	0.749162870
0.346837308	0.846936960	0.749162322
0.153196482	0.499870860	0.749325902
0.000510368	0.653317558	0.749340302
0.846766470	0.847070840	0.749623918
0.652777078	0.499518122	0.749408419
0.499891751	0.653098441	0.749531747
0.319670056	0.486797901	0.916608429
0.167038691	0.180531152	0.916856908
0.013604291	0.333472729	0.916218940
0.820182513	0.486185967	0.916418414

0.667816513	0.179973139	0.916424209
0.513699221	0.332942280	0.916442222
0.320069079	0.986328762	0.916383237
0.166837417	0.680229169	0.916518526
0.013309203	0.832992953	0.916157804
0.819558813	0.985387844	0.917095774
0.665254057	0.679211968	0.916276491
0.513164167	0.832902904	0.917253273
0.166368924	0.333340107	0.021027440
0.668002623	0.331490985	0.020899664
0.168200679	0.835242322	0.020770469
0.664498117	0.831392190	0.022248701
0.000256755	-0.000824619	0.144199675
0.500119904	0.001019824	0.146028612
0.001379659	0.504297084	0.144667143
0.502117947	0.495300168	0.144727631
0.327490603	0.165818754	0.189747416
0.839225645	0.167858915	0.188695532
0.331240956	0.662067675	0.189070912
0.834486159	0.670835466	0.187221281
0.666455152	0.333351884	0.311435096
0.167936756	0.833818326	0.312812588
0.666306429	0.833747494	0.312606868
0.001002854	0.002034633	0.351137798
0.500006041	0.000241760	0.353194497
-0.000668255	0.499706958	0.352531691
0.499710146	0.499749322	0.352549475
0.331530192	0.165668880	0.477846628
0.833454290	0.168630931	0.478335196
0.334903767	0.666244150	0.478290910
0.833714982	0.667521161	0.478866319
0.166315113	0.333032303	0.523679810
0.665806602	0.333962822	0.519917896
0.166648220	0.832383340	0.520278133
0.668065375	0.834594274	0.520142145
-0.000325754	-0.000766795	0.646318897
0.500077447	0.000049556	0.645522058
-0.000624456	0.500324245	0.646067056
0.500806894	0.500690523	0.646028510
0.333492159	0.166675933	0.686949417
0.833172649	0.166576008	0.687190936
0.333374664	0.666681119	0.687027419
0.833266751	0.666637442	0.687196003
0.166550787	0.333262467	0.813037381

0.666691076	0.333242238	0.812987522
0.166887068	0.833537458	0.812783168
0.666567758	0.832864219	0.813273340
0.000388045	0.000413764	0.854576148
0.500451652	-0.000055706	0.854174564
0.000299661	0.500023312	0.853915140
0.499030067	0.498867389	0.854039467
0.334264937	0.166672313	0.981216593
0.834312925	0.165884663	0.980193834
0.332706321	0.666461353	0.980170127
0.832386102	0.666417166	0.978762666
0.166070669	0.334187763	0.320781021

Interpolating coordinate: 0.483 (-829.727 eV)

0.180295955	0.013531107	0.082648459
0.332803684	0.319663505	0.083574066
0.488936737	0.166132277	0.082150816
0.680988393	0.013180510	0.084397182
0.835571398	0.321460724	0.085735346
0.985700910	0.170888724	0.083140567
0.179793987	0.513879651	0.083815839
0.333274544	0.818793929	0.084066967
0.483925677	0.662774109	0.086044162
0.680559465	0.511208838	0.083051167
0.827531352	0.812773060	0.082984481
0.986837177	0.668297964	0.083210607
0.154527019	0.176304254	0.260570544
0.015763523	0.343558008	0.258830354
0.347700128	-0.000019078	0.250912263
0.655809642	0.153508264	0.250338749
0.503611623	0.352215851	0.250292641
0.845538876	-0.001566725	0.250021079
0.152082899	0.652829524	0.249616027
0.001512301	0.848579594	0.251762333
0.325328931	0.483762151	0.258689850
0.649174696	0.651705120	0.249562791
0.497862911	0.843968431	0.250784493
0.849946509	0.499127711	0.249234818
0.021561466	0.191473583	0.411320781
0.309265124	0.332508677	0.410957490
0.168131436	0.477777216	0.410066432
0.512499995	0.180968286	0.415787896
0.819636247	0.334295590	0.416373597
0.666207307	0.486961210	0.416515408

0.014050552	0.678991870	0.416982255
0.319811154	0.832054171	0.416547268
0.166227065	0.986272752	0.416243853
0.514238820	0.680207908	0.416552224
0.820975743	0.835249043	0.416443091
0.667565048	0.987718209	0.416490834
0.484098369	0.320243684	0.581045453
0.179483871	0.165854381	0.582507025
0.333453791	0.013900957	0.582259221
0.986194178	0.320552053	0.582602121
0.680259806	0.166975092	0.582364818
0.835814399	0.016000563	0.581517669
0.486391305	0.819624144	0.582380995
0.180004605	0.664063339	0.581206215
0.333951767	0.513656304	0.582409002
0.986837922	0.819566902	0.583129897
0.680788872	0.667584763	0.583089103
0.832594409	0.513481283	0.583108004
0.346618489	0.346776962	0.749324605
0.153333773	0.000184676	0.749582801
-0.000019902	0.153126189	0.749623439
0.846842396	0.346876464	0.749463370
0.653081355	-0.000508362	0.749427705
0.500347908	0.153253375	0.749161896
0.346843881	0.846934195	0.749160022
0.153202065	0.499866054	0.749329656
0.000512642	0.653310024	0.749336125
0.846766397	0.847071371	0.749625659
0.652782940	0.499525782	0.749414914
0.499897302	0.653100916	0.749541865
0.319680474	0.486798043	0.916607214
0.167060910	0.180535200	0.916845529
0.013606146	0.333452609	0.916233876
0.820197529	0.486192820	0.916418134
0.667854073	0.179979434	0.916404302
0.513721664	0.332949280	0.916443999
0.320063303	0.986313916	0.916370806
0.166843609	0.680213957	0.916512560
0.013295338	0.832961740	0.916126518
0.819572414	0.985391184	0.917098646
0.665277070	0.679225917	0.916305884
0.513184179	0.832909081	0.917264469
0.166409342	0.333333669	0.021014609
0.668024176	0.331501094	0.020894551

0.168186689	0.835204920	0.020743837
0.664509702	0.831396195	0.022267315
0.000337531	-0.000731295	0.144232423
0.500088071	0.001021739	0.146013512
0.001408601	0.504289948	0.144671920
0.502090419	0.495233188	0.144747611
0.327434726	0.165736273	0.189759408
0.839159717	0.167843341	0.188714213
0.331259614	0.662070155	0.189074170
0.834452349	0.670772539	0.187228204
0.666429538	0.333369773	0.311439800
0.167942342	0.833836979	0.312790146
0.666292491	0.833734292	0.312611147
0.000983596	0.002074973	0.351182205
0.499990853	0.000230720	0.353185093
-0.000679776	0.499720438	0.352538246
0.499696757	0.499726039	0.352545852
0.331525670	0.165674225	0.477835374
0.833421996	0.168635274	0.478347622
0.334899075	0.666238100	0.478286000
0.833712443	0.667528079	0.478874049
0.166298552	0.333028169	0.523678739
0.665803207	0.333973219	0.519917744
0.166651896	0.832385486	0.520267881
0.668057576	0.834594152	0.520141413
-0.000328238	-0.000767190	0.646315526
0.500072368	0.000046604	0.645518975
-0.000623719	0.500328030	0.646068923
0.500805737	0.500693197	0.646030644
0.333493759	0.166677793	0.686942936
0.833173114	0.166574593	0.687195570
0.333377672	0.666675903	0.687026913
0.833270071	0.666640644	0.687196853
0.166563326	0.333256300	0.813034851
0.666691506	0.333238957	0.812983157
0.166890365	0.833534240	0.812769944
0.666576442	0.832870510	0.813280184
0.000402396	0.000417644	0.854570047
0.500454193	-0.000058798	0.854174086
0.000307867	0.500007447	0.853914869
0.499050832	0.498875594	0.854048056
0.334287998	0.166660849	0.981240107
0.834302586	0.165867988	0.980192907
0.332718340	0.666459033	0.980175283

0.832422540	0.666423570	0.978759006
0.166016296	0.334174617	0.320769297

Interpolating coordinate: 0.500 (-829.736 eV)

0.180124791	0.013435280	0.082564977
0.332816791	0.319660670	0.083551553
0.488989289	0.166088539	0.082071061
0.681007367	0.013187724	0.084399959
0.835607906	0.321432923	0.085729924
0.985752202	0.170772068	0.083163452
0.179799319	0.513851661	0.083812627
0.333264620	0.818771511	0.084054717
0.483955453	0.662774115	0.086054007
0.680617579	0.511284284	0.083050415
0.827718634	0.812988575	0.083017196
0.986829258	0.668273655	0.083203682
0.154306357	0.176244002	0.260566563
0.015711217	0.343573585	0.258826933
0.347721893	-0.000104037	0.250901316
0.655796603	0.153522512	0.250337094
0.503709876	0.352364492	0.250315824
0.845504936	-0.001568199	0.250022823
0.152081677	0.652834949	0.249607664
0.001559367	0.848719260	0.251680143
0.325289073	0.483735497	0.258679574
0.649223041	0.651759317	0.249557399
0.497873362	0.843950364	0.250779891
0.849955003	0.499160306	0.249239042
0.021512655	0.191482942	0.411350811
0.309218697	0.332473701	0.410936968
0.168114854	0.477776229	0.410061350
0.512491411	0.180970191	0.415782189
0.819633265	0.334313374	0.416383037
0.666204172	0.486971674	0.416536321
0.014039783	0.679022871	0.416958086
0.319794753	0.832044025	0.416545883
0.166224046	0.986280590	0.416228596
0.514230662	0.680203232	0.416550251
0.820974261	0.835250541	0.416447683
0.667555639	0.987718300	0.416493585
0.484091218	0.320245771	0.581044508
0.179478543	0.165853991	0.582503880
0.333451338	0.013901235	0.582253783
0.986189248	0.320553027	0.582614493

0.680252747	0.166981126	0.582370989
0.835802482	0.015996264	0.581525418
0.486384581	0.819618348	0.582382343
0.179999241	0.664061785	0.581201140
0.333947506	0.513651642	0.582407846
0.986843396	0.819571926	0.583127723
0.680787851	0.667590810	0.583096269
0.832597650	0.513488653	0.583111190
0.346629324	0.346780693	0.749324460
0.153334933	0.000183363	0.749574779
-0.000017132	0.153125252	0.749625352
0.846848081	0.346877897	0.749466524
0.653079508	-0.000513295	0.749430485
0.500347280	0.153251915	0.749160921
0.346850453	0.846931430	0.749157722
0.153207647	0.499861248	0.749333410
0.000514915	0.653302490	0.749331947
0.846766324	0.847071903	0.749627400
0.652788803	0.499533441	0.749421408
0.499902853	0.653103391	0.749551984
0.319690892	0.486798184	0.916606000
0.167083130	0.180539249	0.916834150
0.013608001	0.333432490	0.916248813
0.820212545	0.486199673	0.916417854
0.667891632	0.179985730	0.916384395
0.513744107	0.332956279	0.916445776
0.320057527	0.986299069	0.916358376
0.166849801	0.680198745	0.916506594
0.013281474	0.832930527	0.916095232
0.819586015	0.985394525	0.917101518
0.665300083	0.679239867	0.916335277
0.513204190	0.832915257	0.917275666
0.166449759	0.333327232	0.021001778
0.668045729	0.331511203	0.020889438
0.168172698	0.835167518	0.020717205
0.664521288	0.831400201	0.022285930
0.000418308	-0.000637972	0.144265171
0.500056238	0.001023654	0.145998413
0.001437543	0.504282813	0.144676697
0.502062891	0.495166208	0.144767591
0.327378848	0.165653792	0.189771400
0.839093789	0.167827767	0.188732894
0.331278272	0.662072635	0.189077428
0.834418539	0.670709612	0.187235126

0.666403924	0.333387662	0.311444503
0.167947928	0.833855633	0.312767704
0.666278553	0.833721090	0.312615425
0.000964338	0.002115313	0.351226612
0.499975666	0.000219680	0.353175690
-0.000691297	0.499733918	0.352544801
0.499683368	0.499702756	0.352542229
0.331521149	0.165679569	0.477824119
0.833389702	0.168639618	0.478360047
0.334894382	0.666232050	0.478281090
0.833709904	0.667534997	0.478881779
0.166281991	0.333024035	0.523677668
0.665799813	0.333983616	0.519917592
0.166655572	0.832387633	0.520257628
0.668049776	0.834594029	0.520140681
-0.000330722	-0.000767585	0.646312155
0.500067288	0.000043651	0.645515891
-0.000622982	0.500331815	0.646070790
0.500804580	0.500695872	0.646032778
0.333495360	0.166679654	0.686936454
0.833173579	0.166573177	0.687200203
0.333380681	0.666670687	0.687026408
0.833273391	0.666643846	0.687197702
0.166575865	0.333250133	0.813032320
0.666691936	0.333235676	0.812978792
0.166893661	0.833531022	0.812756719
0.666585126	0.832876802	0.813287028
0.000416748	0.000421524	0.854563946
0.500456735	-0.000061890	0.854173608
0.000316073	0.499991582	0.853914598
0.499071598	0.498883798	0.854056645
0.334311059	0.166649384	0.981263621
0.834292247	0.165851314	0.980191980
0.332730358	0.666456714	0.980180440
0.832458978	0.666429974	0.978755346
0.165961923	0.334161472	0.320757573

Interpolating coordinate: 0.667 (-829.814 eV)

0.178413152	0.012477011	0.081730160
0.332947862	0.319632318	0.083326424
0.489514815	0.165651164	0.081273514
0.681197112	0.013259860	0.084427731
0.835972989	0.321154917	0.085675703
0.986265127	0.169605509	0.083392299

0.179852640	0.513571758	0.083780502
0.333165376	0.818547334	0.083932218
0.484253214	0.662774176	0.086152456
0.681198724	0.512038748	0.083042891
0.829591459	0.815143731	0.083344343
0.986750071	0.668030569	0.083134432
0.152099732	0.175641483	0.260526754
0.015188158	0.343729351	0.258792724
0.347939546	-0.000953624	0.250791848
0.655666213	0.153664994	0.250320545
0.504692402	0.353850897	0.250547657
0.845165532	-0.001582936	0.250040262
0.152069461	0.652889203	0.249524038
0.002030032	0.850115915	0.250858238
0.324890487	0.483468952	0.258576819
0.649706491	0.652301292	0.249503482
0.497977872	0.843769692	0.250733872
0.850039945	0.499486252	0.249281278
0.021024545	0.191576533	0.411651110
0.308754422	0.332123945	0.410731745
0.167949037	0.477766356	0.410010525
0.512405571	0.180989240	0.415725118
0.819603449	0.334491219	0.416477432
0.666172826	0.487076311	0.416745453
0.013932093	0.679332880	0.416716395
0.319630747	0.831942569	0.416532031
0.166193856	0.986358967	0.416076027
0.514149087	0.680156473	0.416530518
0.820959437	0.835265522	0.416493606
0.667461546	0.987719212	0.416521096
0.484019712	0.320266640	0.581035059
0.179425267	0.165850094	0.582472426
0.333426807	0.013904010	0.582199400
0.986139948	0.320562766	0.582738209
0.680182161	0.167041463	0.582432699
0.835683313	0.015953279	0.581602909
0.486317337	0.819560386	0.582395824
0.179945602	0.664046242	0.581150390
0.333904890	0.513605020	0.582396283
0.986898140	0.819622169	0.583105987
0.680777640	0.667651283	0.583167930
0.832630060	0.513562349	0.583143046
0.346737677	0.346818000	0.749323013
0.153346537	0.000170237	0.749494555

0.000010564	0.153115882	0.749644481
0.846904933	0.346892231	0.749498060
0.653061041	-0.000562624	0.749458282
0.500340995	0.153237316	0.749151173
0.346916177	0.846903783	0.749134722
0.153263470	0.499813189	0.749370948
0.000537649	0.653227149	0.749290172
0.846765594	0.847077218	0.749644808
0.652847428	0.499610035	0.749486352
0.499958362	0.653128141	0.749653170
0.319795071	0.486799599	0.916593857
0.167305324	0.180579735	0.916720361
0.013626552	0.333231296	0.916398179
0.820362709	0.486268201	0.916415053
0.668267227	0.180048687	0.916185322
0.513968536	0.333026272	0.916463544
0.319999765	0.986150601	0.916234070
0.166911721	0.680046625	0.916446933
0.013142829	0.832618394	0.915782373
0.819722026	0.985427932	0.917130235
0.665530214	0.679379364	0.916629210
0.513404305	0.832977021	0.917387634
0.166853933	0.333262857	0.020873466
0.668261259	0.331612296	0.020838309
0.168032794	0.834793497	0.020450885
0.664637143	0.831440258	0.022472077
0.001226074	0.000295262	0.144592650
0.499737905	0.001042806	0.145847418
0.001726963	0.504211459	0.144724470
0.501787613	0.494496407	0.144967393
0.326820073	0.164828983	0.189891320
0.838434512	0.167672030	0.188919706
0.331464855	0.662097435	0.189110007
0.834080440	0.670080339	0.187304350
0.666147782	0.333566551	0.311491537
0.168003792	0.834042168	0.312543284
0.666139173	0.833589069	0.312658211
0.000771756	0.002518713	0.351670683
0.499823791	0.000109280	0.353081655
-0.000806507	0.499868716	0.352610355
0.499549481	0.499469926	0.352506000
0.331475936	0.165733014	0.477711573
0.833066763	0.168683055	0.478484302
0.334847456	0.666171549	0.478231990

0.833684514	0.667604180	0.478959080
0.166116381	0.332982696	0.523666957
0.665765869	0.334087584	0.519916071
0.166692331	0.832409100	0.520155103
0.667971781	0.834592804	0.520133360
-0.000355561	-0.000771532	0.646278445
0.500016492	0.000014125	0.645485055
-0.000615611	0.500369666	0.646089459
0.500793009	0.500722617	0.646054122
0.333511367	0.166698261	0.686871637
0.833178226	0.166559021	0.687246537
0.333410766	0.666618529	0.687021354
0.833306589	0.666675867	0.687206196
0.166701254	0.333188461	0.813007014
0.666696236	0.333202867	0.812935144
0.166926625	0.833498841	0.812624474
0.666671964	0.832939717	0.813355470
0.000560265	0.000460324	0.854502935
0.500482151	-0.000092809	0.854168827
0.000398133	0.499832932	0.853911891
0.499279255	0.498965841	0.854142536
0.334541671	0.166534736	0.981498760
0.834188859	0.165684572	0.980182710
0.332850543	0.666433518	0.980232006
0.832823360	0.666494015	0.978718743
0.165418194	0.334030018	0.320640332

Interpolating coordinate: 0.833 (-829.863 eV)

0.176701513	0.011518743	0.080895344
0.333078933	0.319603966	0.083101296
0.490040341	0.165213788	0.080475966
0.681386857	0.013331997	0.084455503
0.836338072	0.320876911	0.085621482
0.986778053	0.168438950	0.083621146
0.179905961	0.513291854	0.083748377
0.333066132	0.818323157	0.083809718
0.484550975	0.662774236	0.086250905
0.681779869	0.512793211	0.083035367
0.831464284	0.817298887	0.083671490
0.986670883	0.667787483	0.083065182
0.149893108	0.175038965	0.260486945
0.014665099	0.343885117	0.258758514
0.348157198	-0.001803212	0.250682380
0.655535823	0.153807475	0.250303996

0.505674929	0.355337302	0.250779491
0.844826129	-0.001597673	0.250057701
0.152057245	0.652943457	0.249440412
0.002500697	0.851512570	0.250036332
0.324491902	0.483202408	0.258474065
0.650189941	0.652843267	0.249449564
0.498082382	0.843589021	0.250687853
0.850124888	0.499812199	0.249323515
0.020536435	0.191670125	0.411951410
0.308290147	0.331774189	0.410526521
0.167783220	0.477756483	0.409959699
0.512319731	0.181008288	0.415668046
0.819573633	0.334669063	0.416571827
0.666141481	0.487180948	0.416954585
0.013824403	0.679642888	0.416474705
0.319466741	0.831841113	0.416518180
0.166163665	0.986437344	0.415923459
0.514067512	0.680109713	0.416510786
0.820944613	0.835280503	0.416539529
0.667367454	0.987720124	0.416548607
0.483948206	0.320287510	0.581025611
0.179371991	0.165846198	0.582440972
0.333402276	0.013906786	0.582145017
0.986090648	0.320572505	0.582861925
0.680111575	0.167101801	0.582494409
0.835564144	0.015910294	0.581680400
0.486250092	0.819502424	0.582409306
0.179891963	0.664030700	0.581099640
0.333862275	0.513558398	0.582384719
0.986952883	0.819672411	0.583084251
0.680767428	0.667711756	0.583239591
0.832662471	0.513636045	0.583174902
0.346846029	0.346855307	0.749321566
0.153358140	0.000157112	0.749414331
0.000038260	0.153106511	0.749663610
0.846961785	0.346906566	0.749529597
0.653042573	-0.000611953	0.749486078
0.500334711	0.153222716	0.749141425
0.346981901	0.846876136	0.749111722
0.153319294	0.499765130	0.749408486
0.000560383	0.653151807	0.749248397
0.846764864	0.847082533	0.749662216
0.652906054	0.499686629	0.749551296
0.500013872	0.653152891	0.749754355

0.319899251	0.486801014	0.916581714
0.167527519	0.180620221	0.916606572
0.013645104	0.333030103	0.916547546
0.820512872	0.486336728	0.916412252
0.668642822	0.180111644	0.915986249
0.514192965	0.333096265	0.916481313
0.319942004	0.986002134	0.916109764
0.166973641	0.679894505	0.916387273
0.013004183	0.832306261	0.915469514
0.819858037	0.985461338	0.917158952
0.665760346	0.679518861	0.916923142
0.513604420	0.833038786	0.917499602
0.167258106	0.333198483	0.020745155
0.668476789	0.331713389	0.020787180
0.167892889	0.834419476	0.020184566
0.664752997	0.831480315	0.022658224
0.002033841	0.001228496	0.144920129
0.499419573	0.001061959	0.145696423
0.002016382	0.504140106	0.144772244
0.501512335	0.493826605	0.145167196
0.326261298	0.164004174	0.190011239
0.837775235	0.167516292	0.189106518
0.331651438	0.662122234	0.189142586
0.833742340	0.669451067	0.187373573
0.665891639	0.333745440	0.311538571
0.168059656	0.834228704	0.312318865
0.665999794	0.833457048	0.312700996
0.000579175	0.002922113	0.352114755
0.499671916	-0.000001121	0.352987620
-0.000921717	0.500003513	0.352675909
0.499415593	0.499237095	0.352469771
0.331430723	0.165786458	0.477599027
0.832743825	0.168726492	0.478608557
0.334800529	0.666111047	0.478182889
0.833659124	0.667673362	0.479036381
0.165950771	0.332941357	0.523656245
0.665731926	0.334191553	0.519914551
0.166729089	0.832430567	0.520052577
0.667893786	0.834591578	0.520126039
-0.000380401	-0.000775479	0.646244736
0.499965697	-0.000015400	0.645454219
-0.000608240	0.500407517	0.646108129
0.500781437	0.500749363	0.646075465
0.333527373	0.166716868	0.686806819

0.833182873	0.166544865	0.687292872
0.333440851	0.666566371	0.687016299
0.833339787	0.666707889	0.687214689
0.166826642	0.333126790	0.812981708
0.666700537	0.333170058	0.812891496
0.166959589	0.833466661	0.812492229
0.666758803	0.833002632	0.813423912
0.000703781	0.000499124	0.854441924
0.500507567	-0.000123729	0.854164046
0.000480192	0.499674282	0.853909183
0.499486911	0.499047884	0.854228427
0.334772284	0.166420088	0.981733900
0.834085470	0.165517830	0.980173441
0.332970728	0.666410323	0.980283572
0.833187741	0.666558055	0.978682140
0.164874465	0.333898564	0.320523091

Final coordinate: 1 (-829.880 eV)

0.1749898735305866	0.0105604745156309	0.0800605276942872
0.3332100033989742	0.3195756142277320	0.0828761675266668
0.4905658668174342	0.1647764132582518	0.0796784185607199
0.6815766018853486	0.0134041330779668	0.0844832756772432
0.8367031555004855	0.3205989047440753	0.0855672613467643
0.9872909778186381	0.1672723914719966	0.0838499928468934
0.1799592817457020	0.5130119513696290	0.0837162523619649
0.3329668881635272	0.8180989804458945	0.0836872185133971
0.4848487355809472	0.6627742969720790	0.0863493540176857
0.6823610131805358	0.5135476748993186	0.0830278430014666
0.8333371091922026	0.8194540425500975	0.0839986379272985
0.9865916951910748	0.6675443963855138	0.0829959319826519
0.1476864832006284	0.1744364462063885	0.2604471357921161
0.0141420403748356	0.3440408832819210	0.2587243044660633
0.3483748509065767	0.9973472001437986	0.2505729119376723
0.6554054329784265	0.1539499570520180	0.2502874475678134
0.5066574548494640	0.3568237069233169	0.2510113249397003
0.8444867249434427	-0.0016124091909230	0.2500751401866345
0.1520450283203845	0.6529977103121594	0.2493567858167030
0.0029713625417543	0.8529092254929669	0.2492144270123525
0.3240933166785914	0.4829358631419587	0.2583713099387243
0.6506733916083230	0.6533852418108618	0.2493956471670369
0.4981868917204742	0.8434083494944589	0.2506418333846933
0.8502098303014195	0.5001381447221671	0.2493657508364977
0.0200483246691153	0.1917637165207022	0.4122517101680744
0.3078258726682321	0.3314244333047779	0.4103212975511544

0.1676174025748681	0.4777466106395591	0.409908743170074
0.5122338913187904	0.1810273370715581	0.4156109748953336
0.8195438176104152	0.3348469080536384	0.4166662224072407
0.6661101359595714	0.4872855848245221	0.4171637176974179
0.0137167135954361	0.6799528965169844	0.4162330151314590
0.3193027347752936	0.8317396571628692	0.4165043285027640
0.1661334753517443	0.9865157217145826	0.4157708902197823
0.5139859370597955	0.6800629537108380	0.4164910540041009
0.8209297885598269	0.8352954832999312	0.4165854522995212
0.6672733609880840	0.9877210354059732	0.4165761179300499
0.4838767003252981	0.3203083788347044	0.5810161628531708
0.1793187149639815	0.1658423012064220	0.5824095182937112
0.3333777450345398	0.0139095615845950	0.5820906337731873
0.9860413484502283	0.3205822440679532	0.5829856410862603
0.6800409886410146	0.1671621381727293	0.5825561190727822
0.8354449745664240	0.0158673085871387	0.5817578909342702
0.4861828477517010	0.8194444625566851	0.5824227869869296
0.1798383235047869	0.6640151573102939	0.5810488904137977
0.3338196594669841	0.5135117761962227	0.5823731559808378
0.9870076272026900	0.8197226540751096	0.5830625149127401
0.6807572168112483	0.6677722283991480	0.5833112517736296
0.8326948814052703	0.5137097404324245	0.5832067574314400
0.3469543813060654	0.3468926140290334	0.7493201187194803
0.1533697438512192	0.0001439859832305	0.7493341074755745
0.0000659559856838	0.1530971412080002	0.7496827395123471
0.8470186368891590	0.3469208998101743	0.7495611331788055
0.6530241053076629	-0.0006612813284676	0.7495138741703664
0.5003284268712318	0.1532081156856462	0.7491316776776301
0.3470476249968955	0.8468484884783695	0.7490887220960515
0.1533751169759585	0.4997170714118014	0.7494460239556032
0.0005831169143855	0.6530764660752472	0.7492066219131897
0.8467641337253680	0.8470878485639379	0.7496796236978742
0.6529646796173090	0.4997632226298636	0.7496162401905163
0.5000693819799080	0.6531776403119066	0.7498555401349168
0.3200034307026711	0.4868024294097366	0.9165695715455966
0.1677497133071785	0.1806607066136907	0.9164927831295250
0.0136636552038263	0.3328289095971889	0.9166969122444578
0.8206630351158799	0.4864052557384571	0.9164094504179578
0.6690184166818127	0.1801746003582420	0.9157871764888017
0.5144173934799455	0.3331662579921782	0.9164990819098988
0.3198842430946613	0.9858536664855355	0.9159854588152133
0.1670355602178489	0.6797423858268776	0.9163276116917992
0.0128655382362559	0.8319941283404874	0.9151566546725944
0.8199940480468806	0.9854947444231956	0.9171876687061431

0.6659904775404448	0.6796583587359138	0.9172170747652477
0.5138045344832026	0.8331005501838654	0.9176115693072857
0.1676622800683614	0.3331341078386448	0.0206168426661912
0.6686923195693137	0.3318144810989057	0.0207360508327640
0.1677529838297739	0.8340454544835526	0.0199182460771219
0.6648688522324774	0.8315203717081574	0.0228443705748478
0.0028416070323035	0.0021617295866399	0.1452476074203749
0.4991012410454740	0.0010811115749304	0.1455454282456881
0.0023058012612841	0.5040687525225610	0.1448200169258067
0.5012370575709998	0.4931568040780266	0.1453669981422561
0.3257025225688929	0.1631793647146862	0.1901311593288169
0.8371159580576266	0.1673605541154771	0.1892933293834490
0.3318380203937113	0.6621470341033059	0.1891751644994369
0.8334042402998273	0.6688217945881076	0.1874427967266361
0.6656354958381205	0.3339243285141033	0.3115856052288953
0.1681155194607018	0.8344152392390836	0.3120944461847674
0.6658604152691250	0.8333250263517440	0.3127437809582130
0.0003865932117011	0.0033255130704383	0.3525588256089360
0.4995200409972951	-0.0001115208015478	0.3528935850945848
-0.0010369274586082	0.5001383100512730	0.3527414625696106
0.4992817051552298	0.4990042646084344	0.3524335418367287
0.3313855098894778	0.1658399029199179	0.4774864805202190
0.8324208862350821	0.1687699289502382	0.4787328121388341
0.3347536030694979	0.6660505458502975	0.4781337889360198
0.8336337338641009	0.6677425441520658	0.4791136817614263
0.1657851605296727	0.3329000178363098	0.5236455337515016
0.6656979818628909	0.3342955210361581	0.5199130300621473
0.1667658478231884	0.8324520343488707	0.5199500514075205
0.6678157903251493	0.8345903517917109	0.5201187172874452
-0.0004052403695701	-0.0007794259190554	0.6462110258000010
0.4999149015757459	-0.0000449261874546	0.6454233837252134
-0.0006008687896210	0.5004453678723667	0.6461267981287591
0.5007698654578556	0.5007761084258043	0.6460968086170632
0.3335433797256011	0.1667354742897956	0.6867420022788746
0.8331875199537402	0.1665307090051468	0.6873392059461608
0.3334709368287065	0.6665142129450538	0.6870112452852327
0.8333729853629118	0.6667399106692939	0.6872231828517257
0.1669520310274434	0.3330651183788233	0.8129564019299608
0.6667048369350934	0.3331372494107263	0.8128478482020277
0.1669925529924207	0.8334344803308167	0.8123599846139543
0.6668456415050087	0.8330655469295685	0.8134923544133039
0.0008472969098746	0.0005379239263053	0.8543809137632774
0.5005329830840164	-0.0001546477022634	0.8541592645125072
0.0005622515573460	0.4995156318303774	0.8539064756142306

0.4996945672988957	0.4991299277228050	0.8543143184721078
0.3350028960163721	0.1663054401926678	0.9819690389610712
0.8339820817318018	0.1653510874722732	0.9801641712504955
0.3330909123776841	0.6663871269196087	0.9803351385870656
0.8335521228117346	0.6666220958523733	0.9786455368139547
0.1643307367877172	0.3337671097801522	0.3204058505062150

(2.10) $2 \times 2 \times 1$ supercell with the typical snapshots chosen from ab initio molecular dynamics simulations

Snapshot: 2.5 ps (-825.078 eV)

0.17585612	0.00884191	0.08092728
0.33388650	0.32461342	0.08114028
0.49748034	0.18265400	0.07809961
0.67470423	0.01066992	0.08822624
0.83295344	0.30551373	0.09068044
0.98366117	0.16983677	0.08147168
0.16706411	0.50756958	0.08150383
0.32576316	0.80998693	0.08683848
0.47687077	0.65924328	0.07958930
0.69103157	0.51823515	0.08920515
0.84510483	0.82336558	0.09206845
0.97921486	0.65436593	0.07785480
0.14495510	0.17137759	0.25844036
0.00413481	0.33347985	0.26269552
0.35106401	0.99696688	0.25609387
0.64235217	0.14922517	0.25178375
0.50498349	0.36633057	0.24778339
0.83956656	0.98211519	0.24896980
0.14620373	0.65132104	0.24618031
0.01461429	0.86070000	0.25113062
0.31159787	0.47088911	0.25893178
0.64405697	0.64637780	0.24957781
0.48782130	0.83579688	0.24578767
0.84092923	0.48735427	0.24098212
0.02169276	0.18813898	0.41223132
0.31307764	0.33526963	0.41236007
0.16833202	0.47954944	0.41320752
0.50460174	0.15831579	0.42051136
0.81758971	0.33054555	0.41810964
0.66402315	0.48976000	0.41535116
0.00959369	0.67955677	0.41613738
0.31805361	0.82628240	0.41831361
0.15728182	0.97286355	0.41365101
0.51064235	0.68295234	0.41825138
0.82020852	0.84171728	0.41260069

0.66612141	0.98235631	0.41509468
0.49431305	0.31586239	0.59092787
0.18485279	0.15434432	0.57893633
0.32268760	0.99659602	0.59092351
0.99612666	0.31623393	0.58234500
0.68172443	0.16395973	0.57905919
0.83503525	0.00835252	0.58389701
0.49103608	0.83243973	0.58131062
0.17377668	0.65386446	0.57517503
0.33794644	0.51415223	0.57839676
0.98050894	0.81106718	0.58054356
0.67414157	0.66418958	0.57944504
0.82134401	0.50258250	0.59047585
0.33328639	0.34626505	0.73233375
0.15231864	0.99754473	0.74639960
0.99253100	0.15490949	0.75317162
0.84430345	0.33471438	0.75679710
0.65768050	0.99682324	0.74894321
0.50172888	0.14769321	0.75714612
0.35292128	0.85059966	0.74835460
0.15136459	0.50897673	0.74446329
0.00594010	0.65704690	0.74462714
0.85669617	0.85815969	0.75280396
0.66114067	0.50779323	0.75137896
0.49962436	0.65545903	0.74546922
0.31686253	0.48955597	0.91638087
0.16699548	0.20000024	0.91388852
0.02328069	0.34421851	0.91516596
0.81270636	0.49073775	0.91293839
0.67694310	0.18314138	0.92249427
0.51080960	0.34181435	0.90749726
0.32229500	0.99261710	0.91272761
0.16334335	0.68452137	0.91370426
0.01868929	0.84458552	0.92000796
0.81397674	0.98492404	0.92718283
0.67592098	0.69013966	0.90648687
0.50661316	0.82794208	0.91194692
0.16743247	0.33626300	0.01954131
0.68196304	0.33345714	0.02293049
0.16652475	0.83546377	0.02680870
0.67096872	0.84665925	0.01773318
0.00756590	0.00907835	0.14584326
0.49059146	0.00681190	0.14334291
0.98938689	0.49349846	0.14207952

0.50608520	0.50545118	0.13585867
0.33063458	0.16975524	0.19177845
0.81507644	0.14711784	0.19205237
0.31852508	0.65013567	0.19128504
0.84137917	0.67808572	0.19199125
0.65834986	0.34213999	0.31308434
0.17199341	0.83442911	0.31643207
0.66395851	0.82928510	0.31361609
0.00480246	0.00067008	0.34734512
0.49559587	0.99682971	0.35554662
0.98982360	0.49170400	0.35503510
0.48825364	0.49700468	0.34597413
0.33462133	0.15226739	0.48350219
0.83312937	0.16488832	0.47683849
0.33171432	0.66118700	0.48212335
0.83619137	0.67538608	0.47846168
0.17895476	0.33522847	0.52744813
0.67215454	0.33639140	0.51952943
0.16825232	0.82557460	0.52034377
0.65604065	0.82324299	0.51540806
0.99901853	0.99710990	0.64049337
0.50571017	0.00105936	0.64315332
0.00147239	0.49254364	0.65081017
0.51307753	0.50027376	0.64537270
0.33584000	0.16386382	0.69474068
0.83480284	0.16504366	0.68966994
0.32790337	0.66260708	0.67970157
0.84074659	0.66985223	0.68529906
0.17260614	0.34164165	0.80893274
0.67104663	0.33523891	0.80831482
0.17520082	0.83786558	0.81134606
0.66176142	0.83570104	0.81218861
0.00752384	0.00430544	0.85696028
0.50769450	0.01171366	0.85598837
0.99595386	0.50026374	0.86530918
0.50603145	0.50737798	0.85003185
0.33477890	0.17054352	0.98151268
0.85004765	0.17465437	0.98234596
0.32829189	0.67030750	0.97862270
0.83334078	0.67223344	0.98284011
0.14939059	0.32323955	0.32162576

Snapshot: 5 ps (-825.401 eV)

0.18512782	0.00790973	0.08669184
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0.33582585	0.31593845	0.08569888
0.49607886	0.16984256	0.07761256
0.67677887	0.00892950	0.08284409
0.83102553	0.32112159	0.07691507
0.97982687	0.17720941	0.08251656
0.19185958	0.52235206	0.08206264
0.34002402	0.82443064	0.08111399
0.49496765	0.67129539	0.09497188
0.67493798	0.51537406	0.09274184
0.82339240	0.81277838	0.07569581
0.98301615	0.66542368	0.09062766
0.16945379	0.18662380	0.25948683
0.03330833	0.35455786	0.25064236
0.34151768	0.99555358	0.24386336
0.66582157	0.14578102	0.25929099
0.49459439	0.34314159	0.25326180
0.83689111	0.00305711	0.24998919
0.15573965	0.65692122	0.24895344
0.00218598	0.84972017	0.25606046
0.33797127	0.49495535	0.25919171
0.65399654	0.65199042	0.25744076
0.50352628	0.85356196	0.26006387
0.84380512	0.49736950	0.24639389
0.00965625	0.18186078	0.41769529
0.30219652	0.33828251	0.40888128
0.16913914	0.47341336	0.40954061
0.51285299	0.18070908	0.41784392
0.81905232	0.33619676	0.41173404
0.66801983	0.49255648	0.41468310
0.02080841	0.68331861	0.41812295
0.31756191	0.82092406	0.40670571
0.18141226	0.99562912	0.41202071
0.50697502	0.68834241	0.41473700
0.81908458	0.83337822	0.41647049
0.65568532	0.98525759	0.42103799
0.48169363	0.31462108	0.57585645
0.18161620	0.16151109	0.58157617
0.32035621	0.01277086	0.58447419
0.98418719	0.31881154	0.58571353
0.67560264	0.16122980	0.58153919
0.82755637	0.01034325	0.57631642
0.48385201	0.81636967	0.59057969
0.17918032	0.67372605	0.58621943
0.32338273	0.51126280	0.58088408

0.97785675	0.81580133	0.57940205
0.68096954	0.67824961	0.58454364
0.83826662	0.51541340	0.58371277
0.34855141	0.34285095	0.74820350
0.14759216	0.99749320	0.75627040
0.00561658	0.16443006	0.74413972
0.83986518	0.34292184	0.75218848
0.65274807	0.99163952	0.75301790
0.48855526	0.14829950	0.74900236
0.35688356	0.85619826	0.74924141
0.15835102	0.49914110	0.75347027
0.99584736	0.65307142	0.75786724
0.84806377	0.84940953	0.74258417
0.65374197	0.49908601	0.73863907
0.49527393	0.63642245	0.74877184
0.32457125	0.47594722	0.92363754
0.16198206	0.17233415	0.91776879
0.01630873	0.32680417	0.90791769
0.81564717	0.49050388	0.91080803
0.67068971	0.18085564	0.90898848
0.50578587	0.32337629	0.91349802
0.32706703	0.97746387	0.91817633
0.17115096	0.67799426	0.91652788
0.01419364	0.82541935	0.91927340
0.82494976	0.98568949	0.91450239
0.66512207	0.67099817	0.91573675
0.51873527	0.83251500	0.92016506
0.17940621	0.33441814	0.01890754
0.67251654	0.33172471	0.01146477
0.16816645	0.83263229	0.02408095
0.65943655	0.83205191	0.02563750
0.99849382	0.00581375	0.14386904
0.50160812	0.00453963	0.14205083
0.99773258	0.50098145	0.14072398
0.50242695	0.50451471	0.15459907
0.32815729	0.16442545	0.19011053
0.83768648	0.16213616	0.18873101
0.33348140	0.66506736	0.18460875
0.83375236	0.68231184	0.18700952
0.66952611	0.33412334	0.31062789
0.16701382	0.83524176	0.31071351
0.66600699	0.83847112	0.31833089
0.00114932	0.00479232	0.35742748
0.49690339	0.00984833	0.35231790

0.01002767	0.51184623	0.34876616
0.49285586	0.50958830	0.35474330
0.33573878	0.18047061	0.48209417
0.82510891	0.16644559	0.47558575
0.32750233	0.65339556	0.47906069
0.83395405	0.67060218	0.48013257
0.15323020	0.32701263	0.52760687
0.67027990	0.33362623	0.51800855
0.17378582	0.83083074	0.51444831
0.65974621	0.83130548	0.52311841
0.99340112	0.99602919	0.63779117
0.50482779	0.00749091	0.65217396
0.00167892	0.50385358	0.64969024
0.50153052	0.49732225	0.64008146
0.32387346	0.15669331	0.68413535
0.83817394	0.16995445	0.68897142
0.33757801	0.66819106	0.69099167
0.84035754	0.67120201	0.68919098
0.16977608	0.33070030	0.81336721
0.65978609	0.33648114	0.81235462
0.17061305	0.83391044	0.81419386
0.66704327	0.81415588	0.80936094
0.00158815	0.98784188	0.86073324
0.51063051	0.99707982	0.85595929
0.99997117	0.50157764	0.85671912
0.49573967	0.49725462	0.85399582
0.32947749	0.15748536	0.98283440
0.84474325	0.16182685	0.97712877
0.32445234	0.65328471	0.97419623
0.82188312	0.66664458	0.98161686
0.17345380	0.34521558	0.31548859

Snapshot: 10 ps (-825.276 eV)

0.16873256	0.01114556	0.07749198
0.32984229	0.32651950	0.09072321
0.48082287	0.15423550	0.08692874
0.68166476	0.00340060	0.08384807
0.82387255	0.30725090	0.08296979
0.98861719	0.17821122	0.08651607
0.17593583	0.50844966	0.08571772
0.33305093	0.81170358	0.08304064
0.48789132	0.65589261	0.07872915
0.67924807	0.51033731	0.07593532
0.83131058	0.81966072	0.08092707

0.99033506	0.65977042	0.09250399
0.14553802	0.16842157	0.26058640
0.00813259	0.34350378	0.26283107
0.34565151	0.00868679	0.24255573
0.64301546	0.13729047	0.25382606
0.50505728	0.35743814	0.24789204
0.84502249	0.99903534	0.25039979
0.14456783	0.65319128	0.25259289
0.01965224	0.87359946	0.24643533
0.32295940	0.47583180	0.25552692
0.64957258	0.64822429	0.24897991
0.49332898	0.83633623	0.25238205
0.84147169	0.48029841	0.25004773
0.02655801	0.19126136	0.41515782
0.31244704	0.33127465	0.41318814
0.16997881	0.47545324	0.41109243
0.52004095	0.18401556	0.41054090
0.83167271	0.34583885	0.42226919
0.65800665	0.48583319	0.43058384
0.01739933	0.67912471	0.41735674
0.32322496	0.83762293	0.40742094
0.17636244	0.99491785	0.41773721
0.51099737	0.67985036	0.41125483
0.81390276	0.83065282	0.41947724
0.67135847	0.98463305	0.42230813
0.47460997	0.31409470	0.58664285
0.17341389	0.16505975	0.58348958
0.34004915	0.01706672	0.58241530
0.98981205	0.32813761	0.58448825
0.67384023	0.17609428	0.58557233
0.83975420	0.02223588	0.58319261
0.48460109	0.82652671	0.58018414
0.17832127	0.66042304	0.58174271
0.32943916	0.51620591	0.59298110
0.99594434	0.82406215	0.57764631
0.67403213	0.66260885	0.57547243
0.83258526	0.51943134	0.58513004
0.34722779	0.35523026	0.75315184
0.15221405	0.00393923	0.75344329
0.99125064	0.14839266	0.74964163
0.85426856	0.35161292	0.73407158
0.64657037	0.00927494	0.75406677
0.50074488	0.16676781	0.74681033
0.34690124	0.84668719	0.75355569

0.15785042	0.50994110	0.75067737
0.00485131	0.65822888	0.75132398
0.84336272	0.84962695	0.74996617
0.64885313	0.50306086	0.75506852
0.51198181	0.66813369	0.73832526
0.31988443	0.48955253	0.91199855
0.16601818	0.17421356	0.91625796
0.01612739	0.33507745	0.92328192
0.81370823	0.48335850	0.90857197
0.67304517	0.19759709	0.91313789
0.50038453	0.32986330	0.92450063
0.31957729	0.97925678	0.91491014
0.16583244	0.68490668	0.92629261
0.00424336	0.82729620	0.91903241
0.81807785	0.99713183	0.91236096
0.66301803	0.67687393	0.91943662
0.52228294	0.83550199	0.91607587
0.16632876	0.33503975	0.02508180
0.65298906	0.31725693	0.01942798
0.16045357	0.82626509	0.02775963
0.66537356	0.82648604	0.02744207
0.98500325	0.99181056	0.14803128
0.49748697	0.98853107	0.15092600
0.99289576	0.48907001	0.14086792
0.51110722	0.50179704	0.14013883
0.32423789	0.17368087	0.18353640
0.83776171	0.16184919	0.18703258
0.31870904	0.65291588	0.19052547
0.83222121	0.66209083	0.18956076
0.66026346	0.31743177	0.31020100
0.17744284	0.84352892	0.30314133
0.67033653	0.83129118	0.31384207
0.00852457	0.01085258	0.35311202
0.50116625	0.00029310	0.35363935
0.00264119	0.50575632	0.35424120
0.50502175	0.49955112	0.34982640
0.33727233	0.17292364	0.48196541
0.83586283	0.17481702	0.47791391
0.32825335	0.66513127	0.47401237
0.83786589	0.66476996	0.46761760
0.16312302	0.33545590	0.53328714
0.66842659	0.33819112	0.52785443
0.17796265	0.84206108	0.51481356
0.66117370	0.83460381	0.52324668

0.00745479	0.99744476	0.63999099
0.49068142	0.99933774	0.65039539
0.00118075	0.50760091	0.64529592
0.50360997	0.50180737	0.63947942
0.33511984	0.17954488	0.69525852
0.83195319	0.16090375	0.68511780
0.33567773	0.66941137	0.68715240
0.84013404	0.66690137	0.69247465
0.17286077	0.32474945	0.81967344
0.68799117	0.34199359	0.80573610
0.16051489	0.83717342	0.82024974
0.66586293	0.83951555	0.80993082
0.99188391	0.99978555	0.85122638
0.50711667	0.00516544	0.85351418
0.01593819	0.50537386	0.85121854
0.50602376	0.50118617	0.85306124
0.33199569	0.15289710	0.97246136
0.82947182	0.16760803	0.97686647
0.32995644	0.66338649	0.97696705
0.82657066	0.66223506	0.98323309
0.16627408	0.32991441	0.32329963

Snapshot: 12.7 ps (-824.846 eV)

0.17918210	0.02178971	0.08563096
0.33457688	0.31509796	0.07937293
0.47650706	0.15533995	0.08158409
0.67782133	0.02401762	0.08925022
0.85437960	0.33707476	0.07814408
0.98657578	0.17625567	0.08908163
0.18634827	0.51196321	0.07466695
0.33598272	0.83038127	0.08803499
0.48186507	0.68060221	0.08431651
0.68949897	0.50945393	0.08465216
0.83376174	0.82511159	0.09153791
0.98979677	0.67356016	0.09411385
0.17419376	0.18732262	0.25945031
0.02480134	0.33991562	0.26560699
0.35104087	0.00619946	0.24663216
0.65308963	0.15682608	0.24663598
0.50319660	0.34555934	0.25191160
0.84184221	0.99699838	0.25073756
0.16007158	0.66103292	0.25374611
0.01251023	0.85427379	0.25206113
0.33204045	0.49656608	0.25929000

0.66699562	0.66506745	0.25403757
0.49335843	0.84999065	0.25811651
0.85524369	0.49803287	0.25138012
0.01364807	0.18985979	0.41448644
0.30649750	0.33240952	0.40883456
0.16775850	0.47427669	0.41101300
0.51789584	0.18622499	0.41764704
0.81355895	0.33392246	0.41286024
0.66666977	0.49844443	0.40888662
0.02206516	0.68797116	0.42222359
0.32083830	0.83517906	0.41604924
0.16941742	0.99650821	0.41304292
0.52783506	0.68505096	0.42039267
0.82844828	0.84477370	0.41592774
0.67146359	0.00340503	0.41469798
0.48925973	0.32590643	0.57527502
0.18437536	0.16608006	0.58017063
0.33306932	0.01382516	0.58397391
0.98753162	0.32668208	0.58172183
0.67875920	0.15907510	0.58468286
0.84052829	0.01287291	0.58544776
0.48700524	0.82422108	0.58117319
0.17749695	0.66187010	0.57825167
0.32939054	0.49968028	0.58053027
0.98524628	0.81364957	0.58714222
0.69588717	0.67998003	0.58336922
0.82519874	0.50839652	0.57955524
0.35110431	0.34455904	0.75073667
0.15091687	0.99608165	0.74493751
0.99712248	0.14413974	0.74834387
0.84163002	0.35222658	0.73815569
0.64780544	0.99824162	0.74882117
0.49247401	0.14566506	0.75856169
0.34661638	0.83883817	0.75320081
0.15440184	0.48768965	0.74623009
0.98457990	0.63570076	0.74422921
0.85585617	0.84804241	0.74722019
0.65573812	0.51124158	0.75005308
0.49800283	0.65717633	0.75420875
0.30659627	0.47801197	0.91428114
0.15656071	0.16888018	0.91659446
0.00264820	0.32039056	0.91113806
0.81716981	0.48470741	0.91512965
0.67552798	0.18183965	0.90862655

0.51714614	0.33636618	0.92322590
0.31116820	0.97997041	0.91842815
0.17021399	0.67987136	0.91188969
0.01748705	0.83260201	0.91912441
0.81660382	0.98164182	0.91469199
0.66749488	0.68180684	0.92125085
0.51872674	0.84756959	0.91834490
0.16763900	0.33514020	0.02962665
0.66246841	0.33375840	0.02014059
0.15795128	0.82866771	0.03131926
0.65956482	0.83762808	0.02781950
0.99404116	0.00239964	0.14972122
0.49743271	0.00166720	0.15185877
0.00998638	0.50854013	0.14402056
0.50800860	0.52347810	0.13748572
0.32582714	0.16583674	0.18689923
0.83113133	0.16950727	0.18569699
0.32788845	0.66207199	0.18786288
0.83300043	0.66164170	0.18951321
0.66295660	0.33285288	0.30919544
0.16749857	0.83683755	0.31659353
0.66458411	0.83101441	0.31464492
0.99287156	0.00902004	0.35266487
0.50112379	0.00562433	0.35786376
0.99744053	0.50255962	0.35337500
0.49929990	0.49739266	0.34628911
0.33393527	0.17123907	0.48225711
0.83239800	0.17312285	0.48176623
0.33267212	0.66380551	0.47579788
0.83029447	0.66272344	0.47592326
0.15937455	0.32197352	0.51783759
0.65910305	0.32988127	0.51934449
0.16453052	0.83524654	0.52307142
0.67544937	0.84262342	0.51730984
0.99969406	0.99850594	0.64510871
0.49904568	0.98718062	0.64720392
0.99904434	0.50091630	0.64181394
0.50769717	0.50378199	0.64326584
0.34364568	0.16945922	0.68830758
0.82898085	0.15937283	0.68551067
0.33356515	0.65387681	0.68998956
0.84004980	0.66210477	0.68105813
0.16495721	0.31917235	0.81561994
0.66058863	0.32552666	0.80503987

0.17204401	0.82856615	0.81290194
0.68120414	0.83497475	0.81050250
0.99757632	0.98831164	0.85338198
0.50075160	0.98997527	0.85562144
0.99843723	0.48470859	0.84146757
0.49500358	0.49755253	0.85808446
0.33237408	0.16431158	0.98195352
0.83149638	0.17398113	0.97534945
0.33288083	0.66594045	0.98438226
0.83621520	0.67317302	0.98145744
0.17879208	0.34109917	0.32243067

Snapshot: 15.5 ps (-825.302 eV)

0.17940601	0.00912219	0.08782599
0.32692611	0.31574615	0.08385999
0.48884938	0.16718955	0.08797120
0.66983299	0.00171563	0.07984027
0.83894009	0.32575911	0.08447012
0.96548634	0.14740775	0.07929678
0.19709739	0.51931795	0.08199334
0.33608235	0.81898231	0.07392744
0.49788365	0.65629741	0.07826170
0.67376497	0.50988590	0.09051826
0.83056922	0.80870281	0.08537522
0.99421832	0.67130821	0.07308992
0.15754774	0.16839982	0.25682619
0.02391838	0.33540385	0.25094999
0.33470222	0.00114597	0.25289999
0.66525476	0.14790150	0.24753472
0.49810453	0.34255742	0.25510670
0.85118622	0.99464192	0.24942941
0.14327978	0.64404986	0.24011942
0.98591051	0.83802182	0.25323304
0.32323247	0.46810059	0.26191483
0.64670226	0.65539550	0.25110562
0.49307562	0.85153182	0.25606244
0.85789078	0.49620460	0.24584033
0.02720097	0.19316234	0.40858367
0.30696504	0.32129244	0.41010665
0.16936044	0.47049165	0.41500100
0.51210435	0.17890562	0.41102847
0.82299304	0.32737281	0.40811003
0.66185268	0.48605498	0.41490535
0.01536036	0.67410894	0.41599645

0.32070512	0.83699642	0.41686314
0.15969444	0.97585166	0.42514824
0.51366337	0.67674330	0.41812510
0.82010753	0.83841508	0.42565424
0.66075486	0.98448804	0.41755347
0.49335432	0.32873516	0.57712837
0.18100000	0.17935899	0.58807474
0.34208737	0.01936916	0.58717713
0.99032173	0.32410051	0.58445049
0.69092312	0.18052480	0.57862187
0.83893198	0.01991686	0.58446654
0.48616166	0.83925343	0.57707861
0.17439028	0.66617839	0.57996630
0.33931563	0.52284457	0.58097969
0.98265209	0.83432681	0.57851068
0.68202633	0.66442517	0.58437092
0.83708604	0.51179139	0.57838795
0.34828001	0.34946295	0.75081658
0.15657459	0.01289102	0.74945606
0.99216749	0.14658038	0.75231541
0.85174353	0.35370133	0.75516642
0.65961732	0.01223874	0.74521542
0.51540302	0.16541161	0.74750506
0.35340448	0.85810393	0.75034563
0.16011995	0.51762484	0.76162094
0.99753926	0.65811172	0.74329997
0.84249715	0.84942167	0.74849286
0.65218572	0.49856633	0.74224288
0.49653772	0.64745832	0.74817626
0.31988895	0.48146615	0.90993996
0.17554969	0.19389609	0.91662375
0.01413685	0.34802720	0.91408312
0.81880791	0.48315874	0.90693086
0.67067085	0.17603265	0.91721291
0.51440552	0.33015975	0.91777278
0.32213253	0.99700521	0.91409893
0.17503763	0.68587025	0.91640141
0.01085283	0.83771263	0.91030611
0.81784285	0.99273271	0.91195516
0.66481450	0.68648670	0.91567404
0.51205661	0.83050365	0.91073695
0.15977853	0.32998968	0.02340619
0.67048734	0.33514244	0.02034452
0.17272338	0.83520869	0.01339090

0.67136757	0.83081330	0.01750048
0.99040769	0.98739928	0.15340364
0.48711870	0.97942958	0.14471183
0.00756859	0.50988983	0.13721000
0.50065779	0.49185105	0.15024004
0.33830498	0.16783824	0.19215948
0.83811484	0.15952535	0.18708097
0.34398637	0.65643478	0.18783261
0.81556545	0.65135710	0.19001270
0.66438993	0.31582969	0.31138028
0.15404514	0.81821701	0.31035575
0.65182437	0.82903964	0.31939752
0.00012411	0.00380217	0.35970947
0.48385665	0.99159895	0.35337864
0.01636922	0.50209036	0.34625813
0.49371271	0.49426095	0.35647160
0.32406000	0.15718353	0.48295474
0.82497022	0.16683663	0.47526461
0.33370863	0.67530863	0.48175725
0.83812207	0.66618877	0.48093662
0.15938932	0.33674254	0.52303514
0.66291362	0.33825761	0.51360277
0.17452854	0.84130606	0.52064493
0.67202188	0.83036499	0.52764167
0.00359638	0.00988607	0.64198252
0.51063371	0.01212313	0.64374563
0.99539389	0.49959027	0.64870679
0.49844697	0.50501614	0.64481116
0.35399215	0.18327726	0.69594261
0.84133667	0.17375313	0.68555577
0.33828160	0.67002564	0.69664590
0.83457589	0.67938438	0.68896361
0.16129140	0.33121657	0.81564432
0.67486865	0.34303127	0.80939714
0.15945364	0.83188613	0.80979595
0.66595037	0.83667449	0.80811871
0.00464529	0.01106027	0.85181146
0.49356276	0.99595210	0.85130171
0.00913370	0.51221664	0.85341361
0.50527560	0.50438504	0.85368720
0.33582792	0.16415939	0.98377619
0.82072745	0.15875073	0.98877984
0.33291697	0.66224286	0.97711753
0.83128991	0.66393232	0.97939305

0.16487055 0.32410594 0.31573148

Snapshot: 18.5 ps (-825.954 eV)

0.16976757	0.00624469	0.07609527
0.32605400	0.30667223	0.08339607
0.48144855	0.16043310	0.08288814
0.67957160	0.01059871	0.08593667
0.82963728	0.31390690	0.08706621
0.98556334	0.16553902	0.08618643
0.17464031	0.50040147	0.08059917
0.32334177	0.81416927	0.08475583
0.46851506	0.65909909	0.08524108
0.69523968	0.50710124	0.08248491
0.82477420	0.81502536	0.08360552
0.99886545	0.67404403	0.08968898
0.16362184	0.17489037	0.25061815
0.00809779	0.34735806	0.25610714
0.35134328	0.99652150	0.24657551
0.65605854	0.14359002	0.25680196
0.50377995	0.34844523	0.24867954
0.85219569	0.99193579	0.24729675
0.15115085	0.64972807	0.24366797
0.00632497	0.84633552	0.24793852
0.32199225	0.48543818	0.26200560
0.65514939	0.65195326	0.24845582
0.49284812	0.83469468	0.25125964
0.84663594	0.48754628	0.25038091
0.03321215	0.20050932	0.40677704
0.31351673	0.34090062	0.41048351
0.16709596	0.47728586	0.41143164
0.51690617	0.18329795	0.42019242
0.83134571	0.34688803	0.41957313
0.65653014	0.48129159	0.41523905
0.01392301	0.68323362	0.41916636
0.32072249	0.83684624	0.42113627
0.16513105	0.99000622	0.42389118
0.52365516	0.68610102	0.41273495
0.82466414	0.83646074	0.40810645
0.66730859	0.98931247	0.41854148
0.47760474	0.31455396	0.58063293
0.18107512	0.16478424	0.58701436
0.33860112	0.02440112	0.58363342
0.98729316	0.32400147	0.58545404
0.67750068	0.16856118	0.58784348

0.83813731	0.02227012	0.58138645
0.49566803	0.82661449	0.58615591
0.18201472	0.67455421	0.58648439
0.32803510	0.51520156	0.57425496
0.98378512	0.81609845	0.58554330
0.69448349	0.67505731	0.57548051
0.83864774	0.51519587	0.59142811
0.34455338	0.36128782	0.73963096
0.14363065	0.99320895	0.75522585
0.99605237	0.15384296	0.75855417
0.83965152	0.35191432	0.75112287
0.65027175	0.00516280	0.76031754
0.48699604	0.15709018	0.75530253
0.34468354	0.84224543	0.75382492
0.15645626	0.50252714	0.74673260
0.98730718	0.64511326	0.75395975
0.84352949	0.84456087	0.74651536
0.65010727	0.50225617	0.74784394
0.51033100	0.67144298	0.74745649
0.31872621	0.48262335	0.91367882
0.17210187	0.18404572	0.91242932
0.01764825	0.32693529	0.91958394
0.82757127	0.49256810	0.91371988
0.67139602	0.18303310	0.91706166
0.50441637	0.33292770	0.91017939
0.32190610	0.99100831	0.91920918
0.15518172	0.67272858	0.91378528
0.99904692	0.82481364	0.91136986
0.81309196	0.98462807	0.91849458
0.66528745	0.68638482	0.92206150
0.50657393	0.83062053	0.92051968
0.16550630	0.32428186	0.02815825
0.66755857	0.32356328	0.01910064
0.16503196	0.83721022	0.01130350
0.65207913	0.83062126	0.02023329
0.99096038	0.99149685	0.14317397
0.49547634	0.99447949	0.14429213
0.99472508	0.49322352	0.14769997
0.50632725	0.50377430	0.13974135
0.33033756	0.16973643	0.18253624
0.84345246	0.17100164	0.19131535
0.33284033	0.65605395	0.19195878
0.83407059	0.65976922	0.18532581
0.66203547	0.32925393	0.31900294

0.17020299	0.82904500	0.31689259
0.66289054	0.83212575	0.31497323
0.00695859	0.00077056	0.34694896
0.50796327	0.00133236	0.34907181
0.00879304	0.50246427	0.35109205
0.50029654	0.50004444	0.34615701
0.33362895	0.17430072	0.47325835
0.83087651	0.17370930	0.48503159
0.34115912	0.67588709	0.47242625
0.82627304	0.66252024	0.46887620
0.16287956	0.33170030	0.52226649
0.66017565	0.33037743	0.52194381
0.16883603	0.84078031	0.52270792
0.67430743	0.84337849	0.52210549
0.99853173	0.99548236	0.64388064
0.50556662	0.00298946	0.65090042
0.00966671	0.51330583	0.65195272
0.50321749	0.50315977	0.64242360
0.32327855	0.16890201	0.68860458
0.83552840	0.17346597	0.69481528
0.34150878	0.67594324	0.68565463
0.83626723	0.66206321	0.68475677
0.17470288	0.34354652	0.81519655
0.65215476	0.33090756	0.81479099
0.15349323	0.82219153	0.81139621
0.67301348	0.83559478	0.81424722
0.00173971	0.00436976	0.85648733
0.49970874	0.00170620	0.85511779
0.99759092	0.48654269	0.86086089
0.51556281	0.51280003	0.85519144
0.33244272	0.16225619	0.97731473
0.84265793	0.16323578	0.97683961
0.32902643	0.66242102	0.98376796
0.82457457	0.65851880	0.98006818
0.17366147	0.33136747	0.31847680

Snapshot: 20 ps (-825.172 eV)

0.17134157	0.01156901	0.07893865
0.33165799	0.32753465	0.08963277
0.48441686	0.16860203	0.09092322
0.69034870	0.02164183	0.08254276
0.83209765	0.32155052	0.08105524
0.98706489	0.16704272	0.08926161
0.18349230	0.52213105	0.08361474

0.34291526	0.84247736	0.07884360
0.49976993	0.65720239	0.07589740
0.68257584	0.52260443	0.07459996
0.83533997	0.82931180	0.08519401
0.98004052	0.66370305	0.09551937
0.14798343	0.16716475	0.26083506
0.00884977	0.32310462	0.26758095
0.34318586	0.99541246	0.24241024
0.65074445	0.15248167	0.25277510
0.49809949	0.34097607	0.24653805
0.83684413	0.98800642	0.25082468
0.14135481	0.64696791	0.25170010
0.00084104	0.85374681	0.25179149
0.32769258	0.46953856	0.26624327
0.65703491	0.65318056	0.24491800
0.51261296	0.84534946	0.24142890
0.84709595	0.49084164	0.25269504
0.02968300	0.18696933	0.41775982
0.30894253	0.31736508	0.41351258
0.16610840	0.47629140	0.41386153
0.50863793	0.16948409	0.40866387
0.82095835	0.32227802	0.40382582
0.68129308	0.50324351	0.41314054
0.01008801	0.68184037	0.42298575
0.31783400	0.82972100	0.41627537
0.16918515	0.97969834	0.41694325
0.51572262	0.67448811	0.41544768
0.83289548	0.83776696	0.42492731
0.67072631	0.98311162	0.41280955
0.48148192	0.31793497	0.58368734
0.18379835	0.17366141	0.58435673
0.32776255	0.02012628	0.58925129
0.98981687	0.31805472	0.58221566
0.68469546	0.16977625	0.58176374
0.83368852	0.00994709	0.58441026
0.47999219	0.82176362	0.56595714
0.16454476	0.65294893	0.57320435
0.33930733	0.51772385	0.58702512
0.99782686	0.82164148	0.59479133
0.68156997	0.67225676	0.58366176
0.82275709	0.50452997	0.58195929
0.34551222	0.34568412	0.75511401
0.15465483	0.00879840	0.75728979
0.99939159	0.15378179	0.75171630

0.83955449	0.34539665	0.74713230
0.64422294	0.99672006	0.74100173
0.50254829	0.14738215	0.74414672
0.32693362	0.83469017	0.74532470
0.14428270	0.49392636	0.74472386
0.98633105	0.65120737	0.75703680
0.85498625	0.85640563	0.74741651
0.64309685	0.49616323	0.74868545
0.50280019	0.64972024	0.75200780
0.31202254	0.48257860	0.91866511
0.15849706	0.18041647	0.92774253
0.01029999	0.32937621	0.91078421
0.81090946	0.46605326	0.91494923
0.65738897	0.17406925	0.92129602
0.50924663	0.32717203	0.91584828
0.32718566	0.98643673	0.91687340
0.17034074	0.67981523	0.91543692
0.00708823	0.82665375	0.91725903
0.81491392	0.99131476	0.91247397
0.66960605	0.68345178	0.91901614
0.50704569	0.82992128	0.91382014
0.16530174	0.33336709	0.02723415
0.66149179	0.33236867	0.02640647
0.15686997	0.82771208	0.02328372
0.67071571	0.83646967	0.01775248
0.00896437	0.00653205	0.14332100
0.50228998	0.00290624	0.14626041
0.01070569	0.50311052	0.15196005
0.49936629	0.49880862	0.14446911
0.33564976	0.17555666	0.18937057
0.82706585	0.15692244	0.19468229
0.33913127	0.66124204	0.18407619
0.84262454	0.67297015	0.18868689
0.66547517	0.32774181	0.31296186
0.17318160	0.84004164	0.31254919
0.66881235	0.82748550	0.31216864
0.99702135	0.00289576	0.35077294
0.49988874	0.99011482	0.34623634
0.00900645	0.51582042	0.35623905
0.49697079	0.50049527	0.35574936
0.33787376	0.16638700	0.47216536
0.83515256	0.16886595	0.47826979
0.33888383	0.66891272	0.46701069
0.83511382	0.66494944	0.48636693

0.16295007	0.33524333	0.52846431
0.65738994	0.33385274	0.51734548
0.16448721	0.83512682	0.52009275
0.66992277	0.83759614	0.51683598
0.00786287	0.01223013	0.64455516
0.49543758	0.99624533	0.63151105
0.99939244	0.50196226	0.64579464
0.51072755	0.50440034	0.64731145
0.32915879	0.17039688	0.68950210
0.83228340	0.16424128	0.68679343
0.33011269	0.66445482	0.68623503
0.83220763	0.67420357	0.69557662
0.15769776	0.33488584	0.81777249
0.66374159	0.33170327	0.80747757
0.16646475	0.83138636	0.81138784
0.67885801	0.83279452	0.81050215
0.00069488	0.99982689	0.85569421
0.50702082	0.99962376	0.84941855
0.00079486	0.50271098	0.85576573
0.49221936	0.49949672	0.86095242
0.32781442	0.15262706	0.97315150
0.83321711	0.16952682	0.98240282
0.33728061	0.66684753	0.98228540
0.82676255	0.66287017	0.97786627
0.16337180	0.33638228	0.32534078

Snapshot: 22.5 ps (-825.244 eV)

0.18196723	0.02491843	0.08426174
0.31843358	0.30603536	0.08845890
0.48494586	0.16494435	0.08041285
0.68009755	0.01443468	0.08601247
0.84446344	0.31966791	0.07844421
0.00625757	0.17699122	0.08661706
0.17928149	0.51432447	0.07953476
0.32201271	0.81752742	0.08740380
0.48671638	0.67168147	0.08369571
0.68298010	0.51007829	0.07654659
0.83352438	0.82308251	0.08465061
0.99150396	0.68018215	0.08786839
0.15936463	0.16765589	0.25782481
0.02340661	0.33622983	0.25920651
0.34237855	0.99519535	0.24832053
0.64733619	0.14256230	0.25761560
0.48401687	0.33293938	0.26027882

0.83849523	0.99334399	0.24608167
0.15561263	0.65263330	0.24818783
0.99621777	0.84921139	0.25114078
0.32328220	0.47784719	0.26206185
0.65133979	0.64731011	0.24846662
0.49530298	0.84027910	0.24936781
0.84291694	0.49332956	0.24034918
0.02482054	0.19409022	0.41099661
0.30528631	0.32045073	0.40410746
0.16531917	0.47546366	0.41109408
0.51673911	0.17550142	0.42447819
0.82129321	0.32958951	0.41141669
0.67154233	0.48429847	0.41418338
0.02266403	0.68050878	0.41260681
0.31569252	0.82699043	0.40955477
0.16018481	0.98150225	0.42277057
0.52231843	0.67931439	0.41500018
0.81853604	0.82433932	0.41397637
0.66755672	0.98258087	0.41688174
0.48333438	0.33085677	0.57549986
0.18749750	0.17493905	0.58202767
0.34065928	0.02084307	0.58668317
0.98181844	0.32133009	0.57992977
0.66753442	0.16783942	0.58662739
0.83566040	0.01767125	0.57362916
0.48876697	0.81317749	0.58422931
0.18092425	0.67581538	0.58088838
0.33318565	0.53296323	0.57994954
0.97942176	0.81505181	0.57838355
0.69106641	0.67111907	0.57873916
0.83202732	0.50885015	0.57866309
0.34183676	0.34398337	0.74440866
0.15031889	0.00951746	0.74348679
0.00334368	0.15930129	0.74632322
0.84013519	0.34240061	0.75155634
0.65104220	0.00103274	0.75041713
0.49635229	0.16398041	0.75540440
0.35623001	0.84952939	0.74968338
0.14653850	0.50105272	0.75714055
0.99895154	0.66263431	0.74819777
0.85212580	0.85573409	0.74434094
0.66447191	0.52097284	0.76327013
0.49701674	0.65030717	0.74649274
0.32327658	0.48141776	0.91852907

0.16571337	0.17366462	0.91077730
0.00530484	0.32008943	0.91534938
0.81535257	0.48189176	0.92485934
0.65498561	0.17635181	0.91637180
0.51194497	0.33594523	0.91683268
0.31179163	0.98775067	0.91187390
0.16860893	0.68409236	0.91093538
0.00793791	0.82777233	0.91602422
0.82072461	0.99136242	0.91217643
0.66876476	0.69080970	0.91636063
0.51241599	0.83218394	0.90941301
0.17813584	0.33669285	0.01957780
0.66687150	0.33474023	0.02551457
0.15743385	0.83731978	0.02084833
0.66342126	0.83175700	0.02175390
0.99878671	0.00064981	0.14666885
0.49046839	0.99779032	0.14332368
0.00493849	0.49434368	0.13961731
0.49607193	0.49154434	0.14358655
0.32890408	0.16711822	0.19364937
0.83473874	0.16171072	0.18685065
0.33010797	0.65368376	0.19042654
0.83581765	0.66932470	0.18764970
0.66294387	0.32721333	0.31523525
0.15994021	0.82108332	0.31541910
0.66315392	0.82728873	0.30727306
0.99336057	0.99350848	0.35463448
0.49689172	0.99529979	0.35022727
0.99151911	0.48564595	0.35226692
0.50504947	0.49625019	0.35066027
0.32820212	0.16546155	0.48182408
0.82159725	0.16885445	0.47772025
0.34201901	0.67578227	0.47549934
0.84359940	0.66568627	0.47407949
0.16873614	0.32743138	0.51499179
0.67704427	0.34411867	0.52939482
0.17946074	0.83986251	0.52732775
0.67402501	0.83903511	0.52677364
0.01168237	0.99975209	0.63809145
0.50292155	0.99573660	0.65035413
0.99988159	0.50446888	0.65032655
0.49690333	0.51021636	0.64007313
0.34164574	0.17787682	0.69186141
0.84254187	0.16929114	0.68831225

0.32935826	0.66446027	0.69027415
0.83587477	0.67542576	0.68929347
0.17499039	0.33519237	0.81508646
0.66385547	0.33564398	0.81673625
0.16485313	0.83004893	0.80677743
0.66064285	0.83472226	0.81182665
0.99459577	0.00466630	0.84708344
0.49727456	0.00883192	0.85137098
0.99382771	0.49123817	0.85466485
0.50855528	0.50611068	0.85841844
0.33709003	0.17009646	0.98157574
0.83098533	0.16292839	0.98362700
0.33928046	0.67161579	0.98273403
0.82976385	0.66713843	0.98050512
0.16542110	0.33055964	0.32075262

Snapshot: 25.5 ps (-825.534 eV)

0.17212215	0.01072334	0.08352400
0.32240097	0.31643663	0.08772875
0.49009843	0.17002626	0.07823495
0.68114099	0.01933978	0.07803447
0.83099241	0.31940795	0.08491700
0.97701647	0.15618271	0.08180888
0.16961258	0.50324052	0.08594917
0.34057190	0.83026033	0.07398639
0.49023550	0.66021644	0.07417264
0.68610672	0.51622289	0.08085262
0.82501055	0.81707296	0.08465895
0.98613387	0.66852006	0.08689984
0.15184231	0.16376770	0.25836780
0.01212476	0.33878781	0.26326499
0.34550622	0.99662650	0.24342682
0.66155140	0.15983641	0.25008143
0.49941877	0.34517609	0.24914825
0.84867703	0.98817391	0.25068458
0.14859219	0.64561992	0.24588850
0.00523776	0.84806254	0.24954118
0.32143255	0.47350381	0.26521814
0.64369323	0.64905537	0.24672263
0.52323640	0.86101911	0.24438890
0.85182795	0.49599690	0.24576363
0.02286563	0.19129396	0.40284632
0.30984356	0.33064606	0.41414995
0.16821220	0.47622972	0.41823158

0.51411638	0.17206275	0.41517776
0.81323992	0.33936103	0.41946432
0.65610896	0.47936477	0.42390292
0.01862234	0.68344440	0.41372884
0.32523290	0.82810763	0.40296495
0.17406232	0.99214592	0.40825246
0.51970435	0.68013568	0.41690111
0.82024402	0.83263510	0.42290886
0.66520003	0.98127516	0.41228260
0.48990546	0.32658183	0.58869477
0.19347330	0.17066976	0.58016150
0.32782175	0.00549140	0.58546890
0.97434498	0.31553929	0.57948085
0.67589925	0.15742828	0.57765512
0.84058831	0.01921517	0.58020837
0.49902138	0.82278952	0.58820339
0.19119227	0.67631703	0.58518185
0.33258256	0.50962661	0.58551136
0.99387972	0.82458716	0.57713604
0.68157487	0.67571248	0.58894079
0.84108680	0.52214534	0.58627481
0.33827889	0.34966422	0.75380923
0.16519896	0.00505717	0.75256596
0.00746885	0.15288348	0.75060532
0.84059454	0.35109727	0.74236219
0.65361972	0.00692473	0.74951630
0.50217391	0.15718365	0.74329732
0.34657144	0.84997036	0.74623581
0.16399620	0.50612259	0.75186890
0.01023367	0.65644740	0.75172191
0.84755744	0.83888319	0.74818480
0.64935645	0.50541303	0.75365730
0.50080310	0.65583919	0.75273176
0.31640359	0.48674606	0.91932448
0.16632129	0.18537228	0.92390333
0.01707252	0.34260792	0.91644850
0.80851611	0.48035928	0.90992031
0.66600682	0.18249495	0.92318458
0.50628499	0.32722635	0.91026569
0.31128264	0.99071803	0.91545590
0.15630910	0.67041939	0.92268643
0.01319027	0.82483277	0.91551794
0.82501511	0.99111846	0.91604369
0.66119780	0.67938744	0.91790456

0.50148703	0.84098727	0.91377502
0.15612029	0.32543456	0.02554691
0.67062207	0.33737360	0.02209888
0.16635128	0.83123266	0.02695430
0.67588463	0.83184775	0.01693917
0.99949955	0.99571206	0.14456449
0.50259821	0.00084620	0.14197145
0.99761424	0.49806724	0.14368840
0.50720448	0.50992381	0.13502966
0.32874430	0.17323125	0.19176413
0.83166249	0.15607925	0.18260065
0.34133595	0.66586388	0.18414406
0.83570931	0.66758885	0.19314046
0.66523946	0.33976281	0.31341069
0.16943412	0.82377714	0.30663113
0.67362319	0.82816211	0.32484812
0.99998022	0.99597633	0.35501245
0.51117251	0.00040200	0.34419344
0.00273001	0.49828908	0.35314480
0.48951643	0.50263373	0.35611932
0.33756405	0.17069914	0.47654135
0.84539607	0.18085021	0.47778744
0.33292030	0.67028544	0.47433294
0.83722772	0.65961723	0.48374538
0.17198512	0.34160319	0.52838830
0.65856720	0.32305802	0.52881775
0.16962996	0.83551919	0.51500444
0.66905886	0.85011864	0.52302740
0.00764872	0.00258393	0.63872827
0.49844071	0.99598052	0.64364808
0.99981003	0.49453827	0.65074590
0.50299577	0.51154488	0.65714618
0.33279238	0.16963817	0.69112907
0.83700403	0.15736025	0.68856268
0.32839942	0.66482839	0.68633200
0.83832587	0.65933171	0.68418106
0.16167586	0.32723474	0.81665143
0.65525987	0.33512971	0.81282768
0.16331332	0.82695431	0.82041742
0.65500413	0.83529093	0.81174605
0.00142063	0.99497783	0.85421496
0.50259471	0.01896643	0.85402446
0.99607107	0.49933744	0.85317415
0.49216236	0.49200879	0.85482149

0.32601057	0.16418654	0.98113451
0.83176380	0.17101870	0.97537760
0.33072672	0.66815770	0.97697149
0.82687880	0.66277914	0.97316331
0.16067165	0.32682058	0.32246060

Snapshot: 30 ps (-825.711 eV)

0.17022341	0.01024737	0.08621063
0.31682165	0.30102111	0.08522479
0.49704204	0.17034997	0.08474488
0.67686682	0.00791558	0.07693252
0.83226601	0.31435942	0.09164483
0.97467327	0.16389136	0.08605382
0.18267893	0.51955465	0.08162889
0.33557966	0.81844538	0.08196568
0.48355306	0.66715110	0.08684447
0.69218268	0.51540084	0.08949459
0.83291023	0.81533714	0.08003974
0.98802950	0.66972680	0.07750533
0.14972080	0.15809687	0.25943069
0.01834010	0.34114827	0.26006787
0.34812447	0.99575293	0.24794654
0.66570560	0.15843032	0.25214672
0.49567243	0.33980492	0.24963736
0.84286636	0.99293546	0.23760992
0.14925985	0.65948404	0.24549250
0.00123508	0.85272041	0.24877140
0.32256043	0.47228548	0.25358726
0.64793802	0.65501000	0.26416597
0.50730572	0.85168030	0.25400930
0.85455935	0.50450009	0.25448795
0.02004677	0.19384034	0.40453746
0.31321516	0.33401948	0.40556110
0.17299878	0.49197112	0.40835564
0.51919551	0.18464675	0.41693341
0.82155701	0.33171674	0.41839490
0.65915880	0.48821056	0.41476102
0.01323108	0.67904796	0.41930491
0.32805218	0.83328188	0.41420252
0.17771307	0.98590638	0.41440425
0.52087568	0.68939003	0.41711766
0.82397931	0.83831296	0.41626464
0.66584274	0.98788518	0.41543700
0.48105733	0.32202050	0.57835738

0.18474456	0.17245336	0.58028055
0.33673290	0.01852796	0.58379341
0.98905298	0.32298658	0.58315495
0.67952626	0.16026410	0.57997147
0.84621163	0.02188126	0.57516284
0.49891540	0.81996205	0.58895736
0.18178658	0.65641120	0.58047988
0.33297575	0.51104889	0.58757634
0.98733941	0.82653427	0.58214513
0.68346000	0.66880251	0.58668591
0.83011607	0.51406396	0.58030888
0.34721297	0.33516840	0.74799303
0.15582324	0.99605760	0.74821482
0.00511027	0.15608808	0.75213120
0.83167469	0.34573043	0.75411827
0.64059538	0.98909285	0.74546537
0.49236447	0.14503042	0.75190311
0.34331393	0.84024261	0.74390822
0.14419438	0.49256238	0.75294486
0.00616798	0.65998558	0.75328172
0.85288086	0.84651645	0.75404960
0.65223751	0.51030793	0.74547913
0.48699496	0.63933203	0.75155583
0.31753326	0.48919474	0.92476623
0.16697608	0.18339551	0.91976150
0.01321970	0.32727588	0.91271459
0.82874982	0.49723368	0.91093364
0.65947646	0.17718396	0.91761114
0.52316437	0.33494323	0.92164397
0.31003498	0.98550637	0.91639811
0.17463868	0.69311505	0.91407635
0.00406753	0.82878304	0.92122822
0.82307071	0.98890016	0.91328766
0.65810441	0.67149280	0.92476739
0.50635819	0.83627462	0.91164670
0.15690796	0.32282756	0.01948422
0.67832419	0.33731257	0.02179705
0.17380358	0.83412933	0.01814489
0.66605555	0.83129130	0.02454531
0.99752146	0.99519761	0.14142485
0.49747378	0.99621296	0.14870233
0.00398065	0.50843589	0.14120315
0.50251128	0.49562847	0.13585993
0.32736855	0.16668574	0.18816620

0.83913123	0.16444763	0.18845006
0.33636820	0.65843804	0.19173809
0.82072771	0.66368793	0.19348688
0.66832402	0.33589440	0.30936897
0.16890134	0.83075776	0.31520121
0.67537960	0.84179312	0.31629313
0.00694785	0.00541331	0.35288152
0.50475006	0.00074970	0.35355691
0.99772158	0.48698880	0.35243789
0.50139325	0.50606754	0.35050122
0.33329945	0.17668293	0.46947975
0.82482896	0.16262179	0.48100146
0.34650489	0.67761554	0.48285456
0.83372664	0.66804571	0.47593823
0.17027108	0.34075503	0.51993326
0.66782753	0.33595523	0.51736928
0.16466008	0.83203342	0.52462954
0.67721834	0.83911476	0.52119355
0.00374185	0.00628858	0.64485191
0.50164954	0.99737008	0.64542048
0.00337274	0.50919753	0.64506545
0.49571718	0.49193999	0.64552537
0.33867306	0.15953146	0.68364251
0.82312322	0.16833065	0.69488390
0.32674627	0.65684940	0.68580808
0.82988136	0.66194547	0.68366340
0.16357611	0.32357469	0.81558142
0.65628139	0.33593050	0.80792023
0.17424890	0.83502375	0.81460419
0.65362984	0.82417936	0.80450157
0.99617085	0.98960445	0.85902223
0.49215623	0.00832485	0.85471791
0.01068745	0.50149417	0.85804981
0.49038403	0.49994212	0.86169178
0.34324620	0.18163852	0.97561057
0.82515578	0.16480897	0.98272412
0.33207014	0.67348577	0.98745160
0.83396335	0.66872820	0.98257121
0.16522405	0.32737113	0.31647032

Snapshot: 31 ps (-825.513 eV)

0.18006056	0.01245067	0.07880933
0.33989920	0.32523205	0.07744120
0.48700457	0.16695334	0.08097890

0.68433533	0.02123946	0.08850898
0.84057088	0.32308562	0.08430395
0.98111164	0.15727412	0.07943470
0.18986106	0.51920138	0.07975888
0.34285310	0.82957411	0.08114328
0.48874352	0.66505132	0.08950276
0.68398829	0.51792618	0.09053541
0.82529655	0.81031876	0.08191654
0.97729551	0.65715061	0.08589140
0.13953746	0.15939395	0.25684840
0.02182729	0.34015540	0.25499992
0.33769972	0.00475762	0.25303251
0.65930481	0.15364685	0.24594029
0.49887738	0.34602511	0.24300991
0.84921119	0.98891375	0.25199935
0.15511604	0.65084777	0.24935771
0.99558327	0.85244713	0.24531300
0.32030524	0.46339173	0.25864259
0.64660920	0.65605237	0.24732660
0.51104023	0.86159478	0.25457650
0.83892234	0.48276246	0.24530924
0.02383182	0.19403169	0.41320017
0.29810534	0.31719426	0.40864477
0.15709585	0.46775152	0.41706534
0.52054276	0.18428317	0.41705196
0.82512139	0.34132358	0.41066133
0.66151708	0.49353043	0.41020566
0.01309159	0.68400714	0.41504110
0.31776717	0.83063949	0.41013197
0.16895045	0.98983154	0.41786748
0.51399275	0.67487233	0.41532002
0.82033898	0.82901637	0.41084419
0.65769552	0.98373627	0.42163198
0.48229183	0.32529704	0.57988709
0.16696675	0.17398101	0.58978970
0.33403230	0.00544659	0.58383607
0.98580346	0.31966840	0.58095430
0.68053881	0.17341561	0.58874577
0.82376907	0.00633035	0.57924914
0.49270158	0.82298213	0.57766240
0.18552760	0.65882948	0.58104101
0.33909410	0.50869187	0.58727514
0.99638010	0.82701470	0.58092984
0.67488963	0.65883195	0.57809059

0.82915178	0.51700120	0.58787158
0.34755156	0.35070959	0.74829056
0.15549288	0.99989777	0.74956871
0.99262557	0.15971933	0.75567685
0.83952946	0.34252811	0.74929358
0.64531430	0.99333651	0.75436721
0.50505882	0.15493551	0.74506242
0.34676224	0.84933708	0.74750312
0.14381263	0.49596212	0.74826623
0.99714244	0.65201092	0.75622079
0.85095362	0.85527438	0.74576784
0.66377923	0.50664407	0.76076986
0.49408452	0.64373844	0.74930918
0.32278238	0.48526930	0.91494862
0.17408971	0.18651435	0.91117205
0.01545760	0.34544979	0.92254809
0.82676112	0.49546089	0.92162421
0.66945196	0.17845969	0.92537961
0.51903307	0.33402929	0.91856743
0.32627416	0.99093083	0.90934849
0.17935375	0.68434574	0.91492799
0.01415492	0.83809863	0.91688414
0.81862258	0.99824752	0.91401015
0.66296404	0.68824233	0.91955509
0.52189511	0.83748630	0.91997043
0.16478793	0.33424546	0.01545166
0.66625185	0.32845618	0.02514660
0.16491106	0.82968766	0.00890480
0.67257013	0.84160231	0.02545668
0.99227458	0.98843184	0.14372801
0.50552804	0.00154405	0.14818076
0.01237656	0.50484443	0.14633122
0.49828077	0.49889167	0.14776859
0.31385711	0.15880640	0.18606924
0.83385658	0.15686043	0.19449148
0.33614993	0.66085363	0.19125099
0.83143932	0.65645862	0.18716159
0.65824827	0.32918792	0.30838099
0.16864354	0.83219159	0.30433869
0.67055918	0.83244082	0.31552006
0.00814408	0.01058149	0.35495253
0.49566080	0.00316003	0.35150996
0.00503512	0.50704432	0.34985006
0.49560952	0.50090776	0.35022513

0.33543376	0.16530457	0.48222163
0.83945980	0.17154951	0.47400075
0.32496491	0.66015833	0.47571523
0.83629819	0.67472658	0.47763239
0.16516510	0.33262624	0.52603915
0.66985283	0.34258271	0.51398846
0.15850960	0.82066156	0.52558891
0.66456856	0.82714442	0.51919982
0.00043006	0.99493017	0.64591135
0.50245707	0.00112008	0.64085657
0.99389523	0.49215165	0.64374793
0.50925627	0.49257011	0.65268173
0.33230224	0.16450330	0.68717642
0.82719822	0.16398522	0.68466581
0.32734963	0.66319629	0.68529808
0.82640073	0.66044051	0.69165176
0.16586227	0.33629221	0.80909570
0.66934329	0.33487584	0.81350594
0.16750083	0.83377036	0.81271642
0.66971269	0.82959457	0.81280191
0.99711324	0.01410119	0.85582890
0.50986082	0.00647833	0.85544396
0.00542198	0.50965348	0.86212093
0.49917936	0.50339035	0.85415627
0.33604649	0.17090463	0.98094298
0.83677134	0.17508608	0.98483704
0.34603299	0.67452214	0.98254695
0.82618112	0.66631318	0.98538705
0.16490989	0.33160367	0.31973322

Snapshot: 32.1 ps (-825.083 eV)

0.17387302	0.00807187	0.08502975
0.31633780	0.30975980	0.08848070
0.48728096	0.16387995	0.08603035
0.66091352	0.00158549	0.07754973
0.83076754	0.31315378	0.08960855
0.97879119	0.16905961	0.08251423
0.17221964	0.51301759	0.08753111
0.32628861	0.82038254	0.08429942
0.48205382	0.67760000	0.07317577
0.70410142	0.52233548	0.07940515
0.83600720	0.81396305	0.07995755
0.00898097	0.67506113	0.08509027
0.15618669	0.17851400	0.25144761

0.01356155	0.34650950	0.26162853
0.34786192	0.01670784	0.26088647
0.65099803	0.15408853	0.25054746
0.51663547	0.34234432	0.24963361
0.84012379	0.99464213	0.23966949
0.15517784	0.65603415	0.26041672
0.99724330	0.85908182	0.25960164
0.32863394	0.48589044	0.25619708
0.65446610	0.65110727	0.25598100
0.48775846	0.84127740	0.25561762
0.85073284	0.50976176	0.24892145
0.01955378	0.18457194	0.40910424
0.31045684	0.32343814	0.40171461
0.16792254	0.46539519	0.40815345
0.52140047	0.19061864	0.41484722
0.81926977	0.33913885	0.42636398
0.66619979	0.48029597	0.41202244
0.01420895	0.68803350	0.41360852
0.31134744	0.82604738	0.42151174
0.16161963	0.98202695	0.41714897
0.50375602	0.66607803	0.42572198
0.80510418	0.82978042	0.41153104
0.66496207	0.98445726	0.41325097
0.48983114	0.32093138	0.58237593
0.18380934	0.16916684	0.57253167
0.33659398	0.00827266	0.58243995
0.98754710	0.31738699	0.57771486
0.67516705	0.15799098	0.58890694
0.83881957	0.01279896	0.58060901
0.47832920	0.81345427	0.58108436
0.17099211	0.66668248	0.58559340
0.32972914	0.50737310	0.57827714
0.98734770	0.82687101	0.57679358
0.68402989	0.65950562	0.58421343
0.83325141	0.51675612	0.58375302
0.35207969	0.34736959	0.75570849
0.16067898	0.00469074	0.74377702
0.00033565	0.15522880	0.74375453
0.85776225	0.35211921	0.74588606
0.66349985	0.00581151	0.75595493
0.50145680	0.15788987	0.75242543
0.34667087	0.84939321	0.74713073
0.15862763	0.49514330	0.75088823
0.00448757	0.66358380	0.74190961

0.84832302	0.84802268	0.74953708
0.65540286	0.50269072	0.75015824
0.50336341	0.64390800	0.74605165
0.33195339	0.49392057	0.92067750
0.16814782	0.17282649	0.91907549
0.01193246	0.32343498	0.91589579
0.83378283	0.49285250	0.91515821
0.66688982	0.18904527	0.91432954
0.52105989	0.32847711	0.92182392
0.33182230	0.98539105	0.91853591
0.16829984	0.68455902	0.90939705
0.02053996	0.83472935	0.91134387
0.81900442	0.98288579	0.91471611
0.67770006	0.68595428	0.91467524
0.51168915	0.83680887	0.91289015
0.16490248	0.33809652	0.02382801
0.66834676	0.34152897	0.02456601
0.16134350	0.82991532	0.01754831
0.67035348	0.83792655	0.01767435
0.99979407	0.00238899	0.14715775
0.50388770	0.99919349	0.14345822
0.00327421	0.51057414	0.15272356
0.49161255	0.49865713	0.13870137
0.33067832	0.17929185	0.19072050
0.83832605	0.17005901	0.19562187
0.33261071	0.67517508	0.18523600
0.83544710	0.67630049	0.18768180
0.66419588	0.32713691	0.31574017
0.16294379	0.83716071	0.32058612
0.65921253	0.82624237	0.30846252
0.98270384	0.99320521	0.35795993
0.49409209	0.99682952	0.35455923
0.00723685	0.50133832	0.35867701
0.49544499	0.48678055	0.34602705
0.33628847	0.16721473	0.47187208
0.83939832	0.16767669	0.47833278
0.33705401	0.66535780	0.48061808
0.83399677	0.66789464	0.47453814
0.16011944	0.32731777	0.51720905
0.66614232	0.33362323	0.52534544
0.16727000	0.83099658	0.51956014
0.65883668	0.83370611	0.51890982
0.01920650	0.00425452	0.64160983
0.49065595	0.99219592	0.65032973

0.99502162	0.50704181	0.64628775
0.49585956	0.49919228	0.64066246
0.33945644	0.17490173	0.67941665
0.83459804	0.16403734	0.69311583
0.33212621	0.65412000	0.68665457
0.84080685	0.67411731	0.68337085
0.16765744	0.32379246	0.82222737
0.66697738	0.34170624	0.81897144
0.16758016	0.84130226	0.81163994
0.66809210	0.82629396	0.80902370
0.99851970	0.99899840	0.85709313
0.50752721	0.00692893	0.85302255
0.00730087	0.49518733	0.85415781
0.49878562	0.49289811	0.86036693
0.32737691	0.15642753	0.98439754
0.81780729	0.15718324	0.98292883
0.33676121	0.66745884	0.97577798
0.84193460	0.66568318	0.97364223
0.16686940	0.33133414	0.31410652

Snapshot: 38.2 ps (-825.484 eV)

0.18064406	0.02310682	0.08230953
0.34371117	0.31415881	0.08361350
0.49450812	0.15883027	0.08234213
0.66834596	0.00785694	0.07943147
0.83044036	0.31672831	0.08702624
0.98385991	0.16602526	0.08059836
0.18079626	0.50652680	0.09126147
0.32825339	0.81399406	0.08474420
0.48517487	0.67547051	0.08617529
0.68259634	0.52340163	0.07433377
0.84008557	0.82670162	0.07793837
0.99616444	0.67038735	0.06912334
0.15525580	0.18092050	0.25718671
0.01056700	0.34626445	0.25675574
0.33750918	0.99620886	0.25217978
0.64454913	0.14694670	0.25469622
0.51266875	0.35172576	0.24655491
0.84075015	0.99822037	0.25279366
0.15720569	0.65724451	0.24926199
0.00720340	0.85252990	0.25128430
0.32506879	0.47646718	0.25676938
0.64252777	0.64101382	0.25970816
0.49856233	0.85111446	0.25409946

0.84209669	0.48857115	0.24739214
0.02899046	0.20579564	0.41644675
0.31288132	0.33353288	0.41101112
0.17150246	0.47861214	0.41020791
0.51456456	0.17639852	0.42270199
0.82097861	0.33228654	0.41623961
0.65976465	0.47635621	0.41557678
0.00966646	0.68194197	0.41744135
0.31724785	0.83433240	0.42090400
0.16215857	0.99104514	0.42278138
0.51417049	0.67638544	0.41917622
0.82674964	0.83918551	0.42265143
0.65616979	0.98030902	0.42523751
0.48792710	0.32295621	0.58193991
0.18506133	0.16503373	0.58317720
0.33538826	0.01399627	0.58156120
0.99386644	0.32399911	0.58343643
0.68726605	0.17806813	0.59441797
0.82899458	0.01617324	0.58175458
0.48306027	0.81777021	0.58627650
0.16427218	0.65802465	0.57239074
0.33499344	0.52141161	0.58297871
0.98316754	0.82539714	0.58838748
0.67887933	0.66645586	0.57799588
0.82963894	0.50895111	0.58829496
0.34534932	0.34373695	0.74946312
0.15894260	0.00645394	0.75025810
0.00595393	0.14800530	0.74934281
0.84831679	0.33570963	0.75763352
0.65072160	0.99836811	0.74615608
0.49429594	0.14999144	0.74062205
0.34876414	0.84645127	0.75283146
0.15506110	0.50108324	0.74776521
0.98426422	0.64548129	0.75775322
0.85050612	0.85295910	0.74431157
0.65226275	0.49703431	0.75102391
0.49154856	0.64620160	0.74917337
0.32826446	0.49004476	0.92201015
0.17356411	0.19009599	0.92044853
0.01730068	0.33412892	0.92698243
0.81076497	0.48404399	0.91254151
0.65537758	0.17079417	0.91756810
0.51154751	0.33287761	0.91326381
0.31315764	0.97734254	0.92324801

0.16224429	0.65966178	0.90863724
0.02790147	0.83334908	0.91620137
0.83211503	0.98721016	0.91681792
0.66746733	0.67797291	0.90814450
0.52312202	0.83055608	0.91818414
0.17115881	0.33538251	0.01851121
0.66123174	0.33447182	0.01982542
0.17066873	0.84024956	0.02213256
0.66256416	0.82392326	0.02516626
0.99305604	0.99184186	0.14475669
0.49751906	0.99382953	0.14805904
0.00139143	0.50115410	0.13929981
0.51007018	0.51328401	0.15063294
0.34031603	0.17659679	0.19204848
0.83310049	0.16451359	0.19224992
0.32986093	0.66121698	0.18894913
0.83030975	0.66251227	0.19095918
0.67081710	0.32720886	0.31461266
0.16407196	0.83553607	0.31082995
0.66391283	0.82702830	0.31267807
0.00405639	0.00493413	0.35389517
0.50257236	0.99916830	0.35679888
0.99848014	0.50056016	0.34759617
0.49489160	0.49367845	0.35581963
0.34308224	0.17113309	0.48009816
0.83516790	0.17047086	0.48380362
0.32803533	0.67561116	0.48364335
0.82657977	0.65758178	0.47303032
0.16973059	0.32933410	0.51883308
0.66077056	0.33179865	0.52787842
0.15719622	0.84237453	0.52158649
0.66313004	0.83158781	0.52083990
0.00154032	0.00938618	0.63719529
0.50873975	0.00502075	0.63997234
0.99866043	0.50030566	0.65066913
0.49071289	0.50224461	0.64243182
0.33268605	0.16976851	0.68584759
0.84395687	0.16571746	0.68841969
0.33294884	0.66640381	0.68898789
0.82216302	0.67221206	0.68269639
0.16290591	0.32594579	0.81308755
0.65648230	0.33092043	0.81204446
0.16213502	0.81985843	0.81005596
0.67858342	0.84502135	0.80696186

0.01526061	0.00835902	0.85456164
0.51013098	0.99550142	0.85486066
0.99134444	0.49210686	0.85534043
0.50421278	0.51023061	0.84703962
0.34416782	0.16254203	0.97779718
0.83559273	0.16700232	0.97867537
0.32681114	0.66543792	0.97480223
0.83765843	0.66212396	0.97986847
0.16469591	0.34049979	0.31786705