

Supporting Information

Methane activation on metal-doped (111) and (100) ceria surfaces with charge-compensating oxygen vacancies

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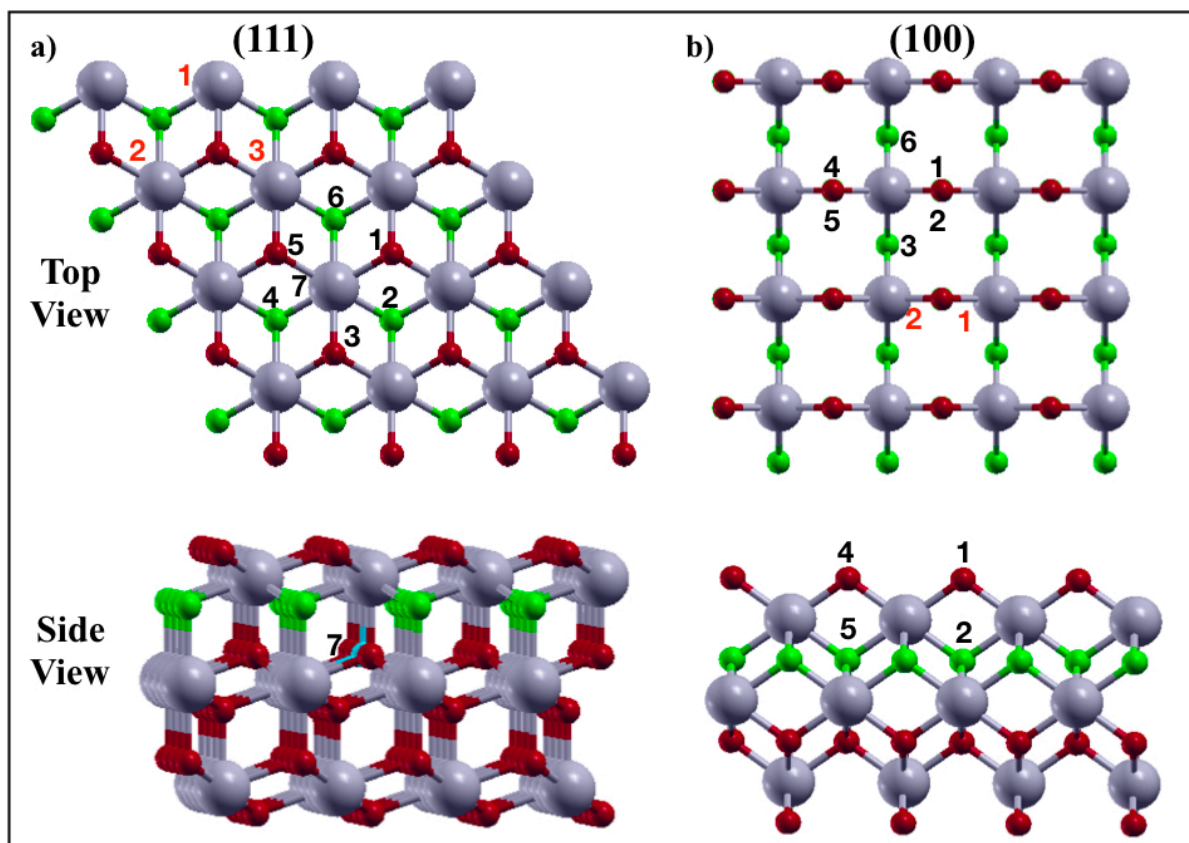


Figure S1 Top and side views of a) CeO_2 (111) and b) (100) surfaces, illustrating the coordination of the surface atoms. Ce atoms are shown in gray, oxygen atoms in red except those of the second layer that are shown in green. Black and red numbers indicate the first neighbors of cerium and oxygen atoms, respectively. For CeO_2 (111), the cyan sphere in the bottom left panel highlights the oxygen of the second trilayer bound to the reference surface cerium atom in the upper left panel.

Table S1 Effect of the coverage (θ) on the computed adsorption energies (eV) of a CH₄ molecule in molecular (MA) and dissociative (DA) forms on pristine CeO₂(111). vdW interactions are not included. Two different coverages are considered: $\theta=1/16$, corresponding to one molecule in a 4x4 surface unit cell, and $\theta=1/9$, corresponding to one molecule in a 3x3 surface unit cell.

CeO ₂ (111)		
	$\theta=1/16$	$\theta=1/9$
MA	-0.04	-0.04
DA	-0.89	-1.01

Table S2 Comparison of computed adsorption energies (eV) for molecular (MA) and dissociated (DA) CH₄ on the pristine CeO₂(111) surface. The symbol * indicates that vdW dispersion is included.

MA	DA	Ref.
-0.38	-1.59	This work*
-0.04	-0.89	This work
--	-0.92	1
<0.05	-0.76	2, 3
-0.21	-1.31	4
--	-1.14	5

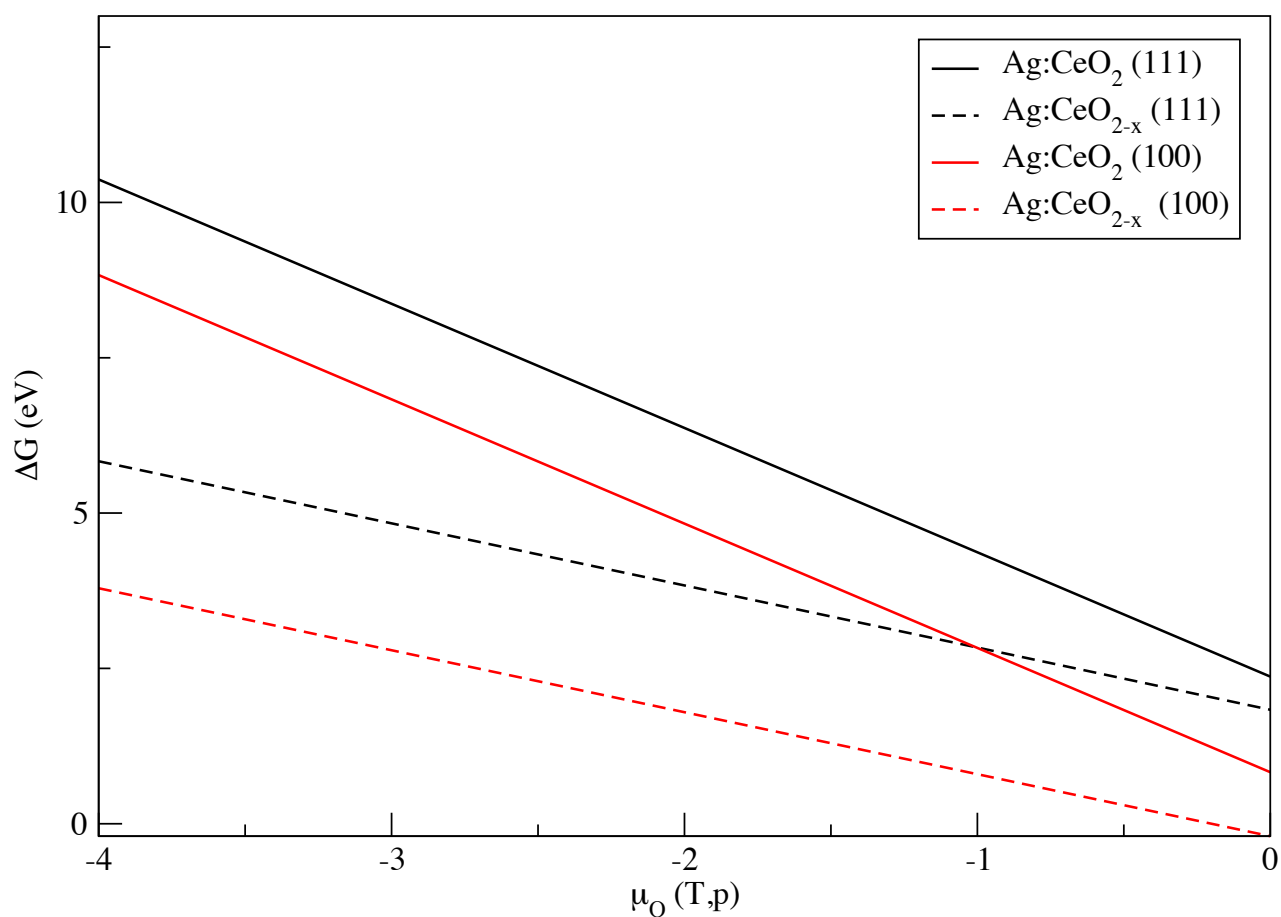


Figure S2 Gibbs free energies of the oxidized and reduced Ag-doped (111) (black lines) and (100) (red lines) surfaces relative to pristine CeO₂(111) and CeO₂(100), respectively, as a function of the Oxygen Chemical potential μ_O (T,p).

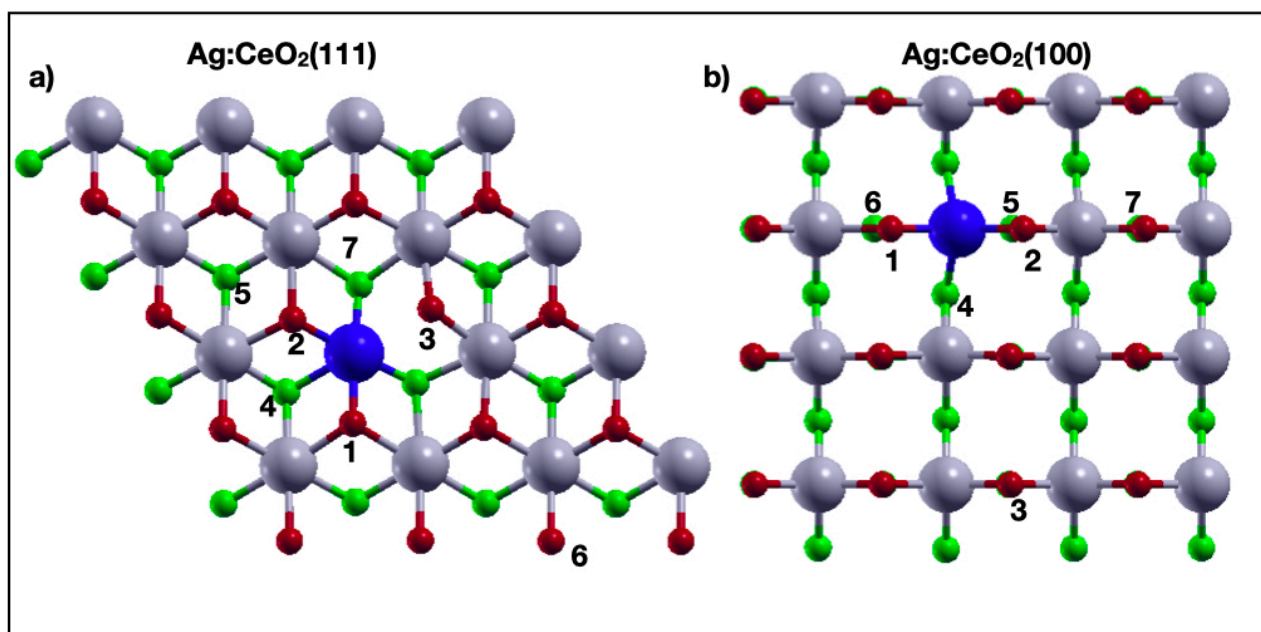


Figure S3 Top views of the a) Ag:CeO₂(111) and b) Ag:CeO₂(100) surfaces. Ce and Ag atoms are shown in gray and blue, respectively; oxygen atoms are in red, except those of the second layer, which are shown in green atoms. Numbers indicate the oxygen sites at which the vacancy formation energy was calculated (see Table 2 of main text).

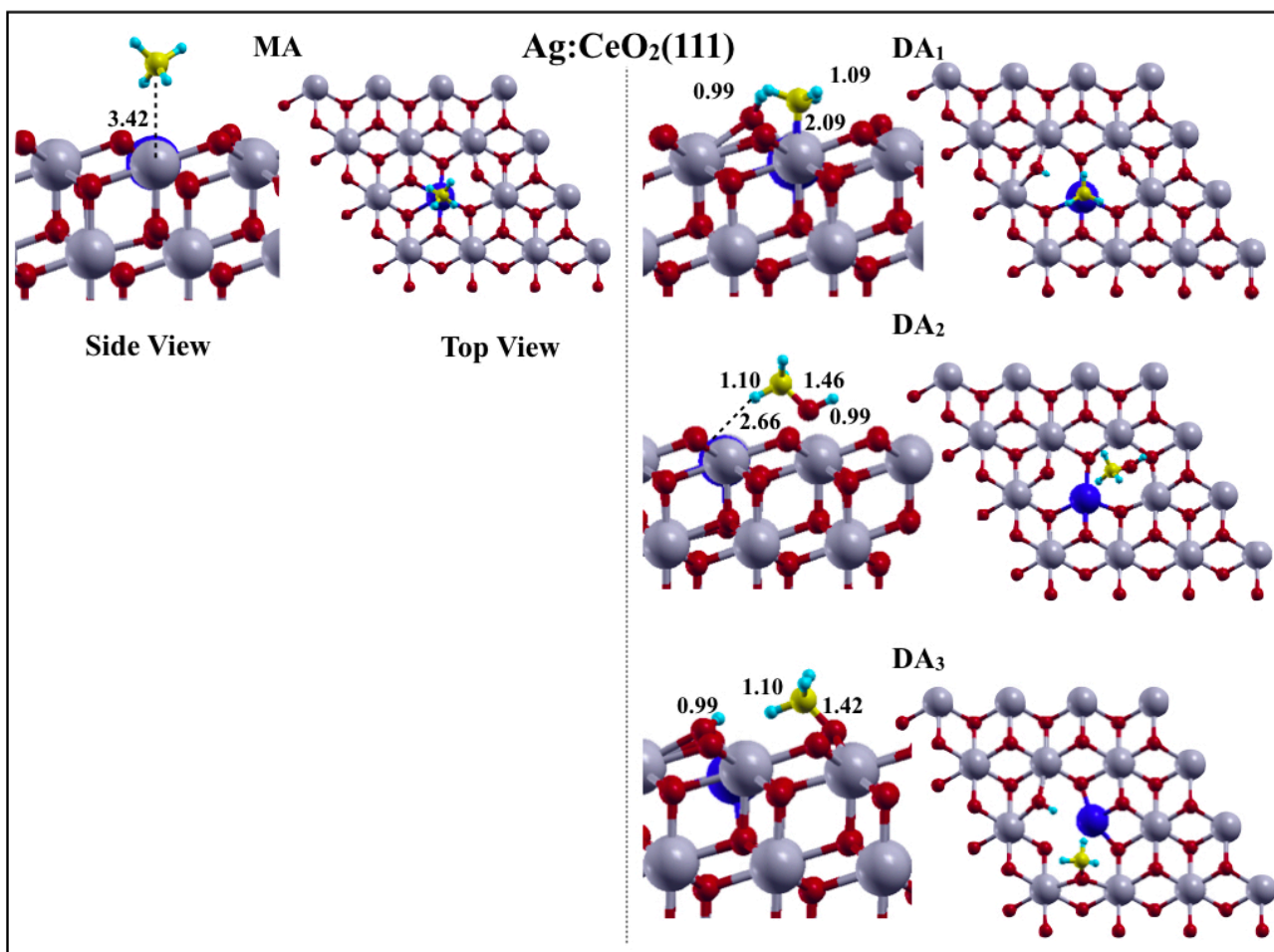


Figure S4 Molecular (MA) and Dissociative (DA) adsorption of CH_4 on the oxidized $\text{Ag}:\text{CeO}_2(111)$ surface. Yellow and cyan balls are the Carbon and Hydrogen atoms. Blue, gray, and red balls represent Silver, Cerium, and Oxygen atoms. No cerium atoms are reduced.

Table S3 Adsorption energy (in eV) of molecular (MA) and dissociated (DA_n) CH_4 on the oxidized $\text{Ag}:\text{CeO}_2(111)$ surface. The structures of the DA_1 , DA_2 , and DA_3 states are shown in Figure S3.

	MA	DA ₁	DA ₂	DA ₃
Ag:CeO₂ (111)	-0.23	-1.57	-2.85	-4.25

Table S4 Adsorption Energy (eV) of CH₄ in molecular (MA) and dissociative CH₃+H (DA₃) forms on the Ag:CeO₂ (111), Ag:CeO_{2-x} (111), and Ag:CeO_{2-x} (100) surfaces. Computed values both with (E_{ads}^*) and without (E_{ads}) long range interactions are presented.

	Ag:CeO ₂ (111)		Ag:CeO _{2-x} (111)		Ag:CeO _{2-x} (100)	
	MA	DA ₃	MA	DA ₃	MA	DA ₃
E_{ads}	-0.03	-3.68	-0.28	-1.92	-0.63	-2.94
E_{ads}^*	-0.23	-4.25	-0.80	-2.45	-1.01	-3.20

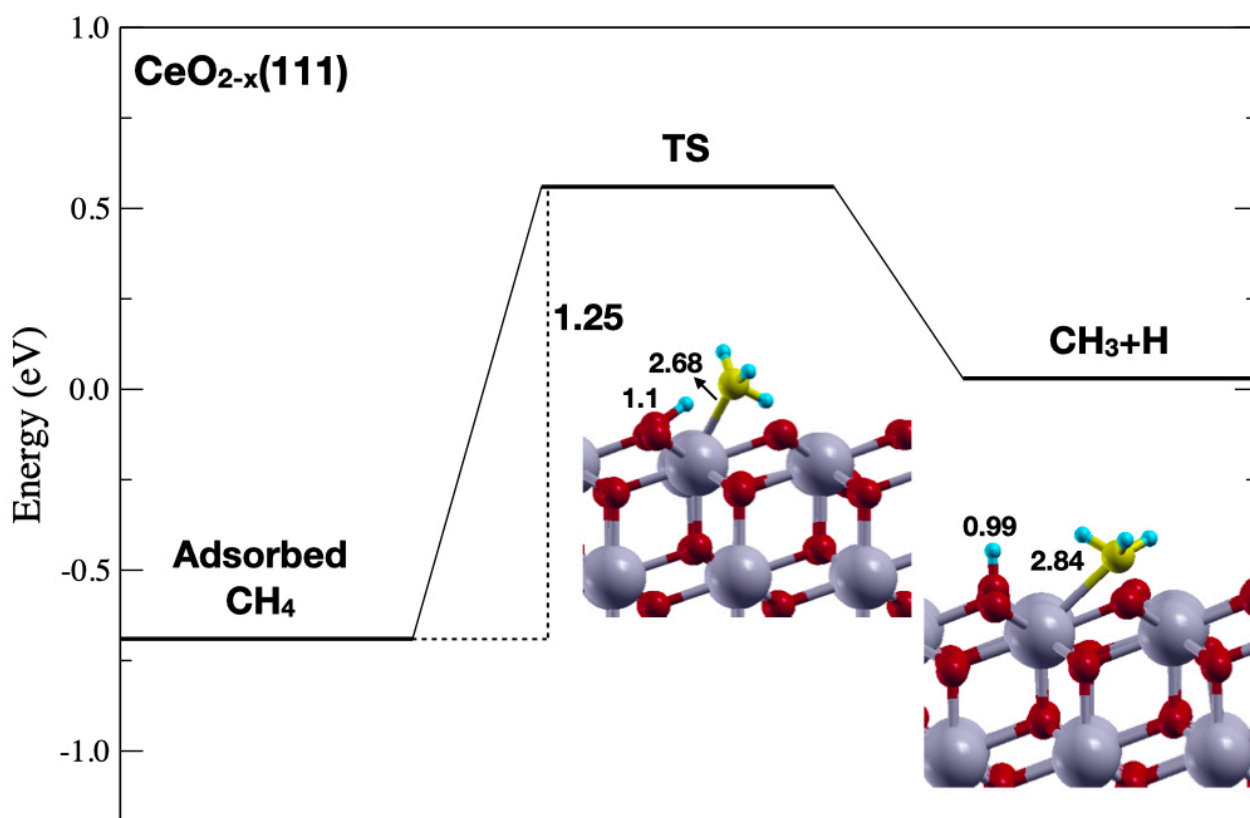


Figure S5 Minimum Energy Pathway (MEP) of CH₄ dissociation on the reduced CeO_{2-x}(111) surface. The oxygen vacancy has been created on the outermost layer to compare the results with those obtained on the reduced Ag:CeO_{2-x}(111) surface. Relevant distances are in angstrom. The energy zero corresponds to the non-interacting surface and gas phase molecule.

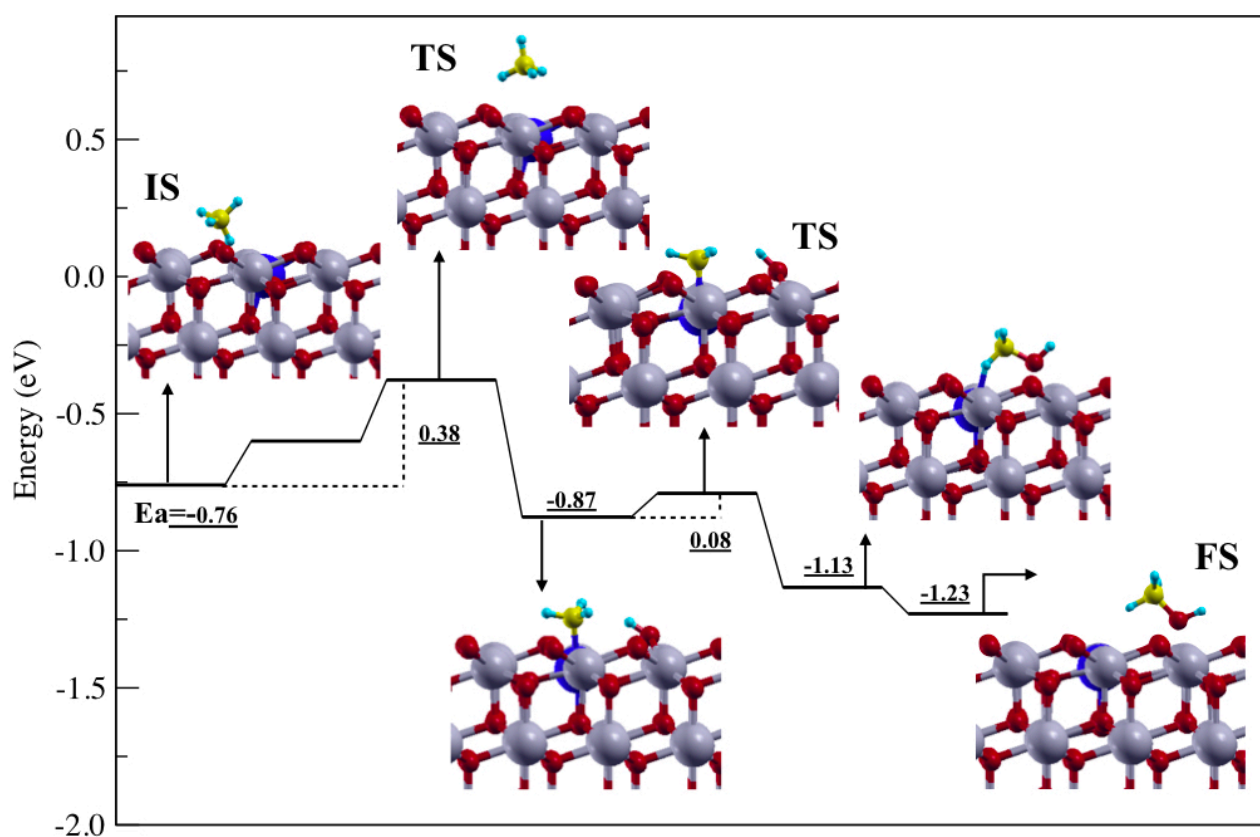


Figure S6 MEP of the dissociative adsorption of CH_4 to form methanol on the $\text{Ag:CeO}_{2-x}(111)$ surface. The reported energies include vdW corrections. All distances are in Angstrom. Ag, Ce and O atoms are shown in blue, gray and red, respectively. Hydrogen and carbon atoms are light blue and yellow, respectively.

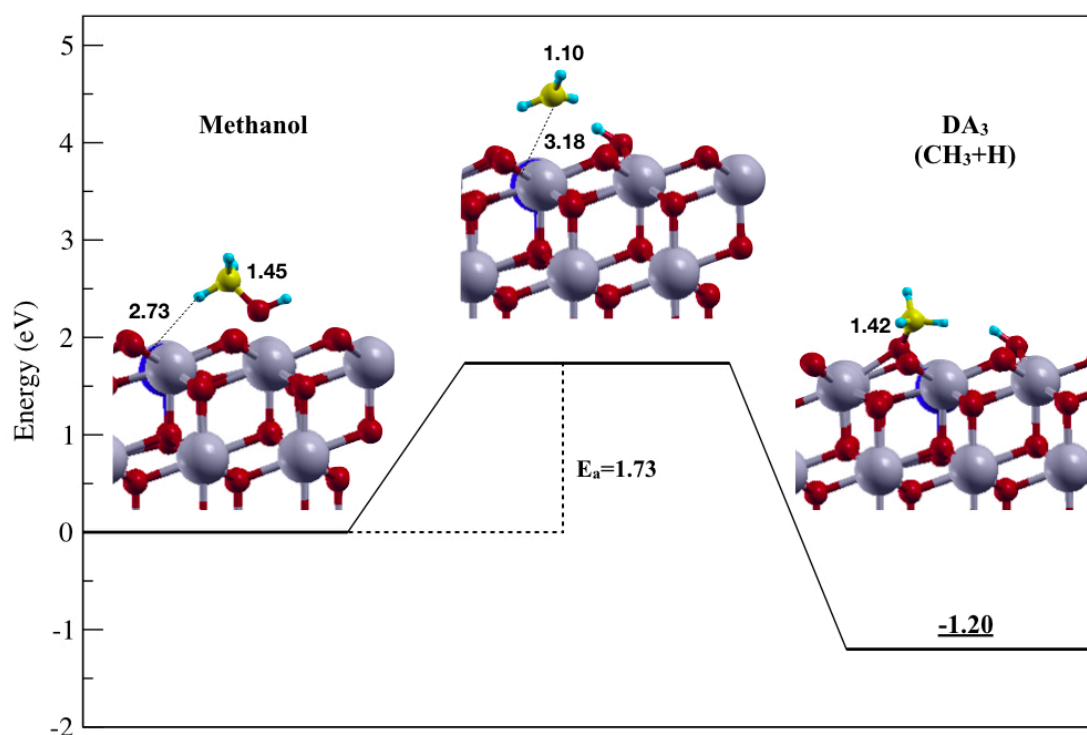


Figure S7 MEP of the reaction $\text{CH}_3\text{OH} \rightarrow \text{CH}_3 + \text{H}$ (i.e. $\text{DA}_2 \rightarrow \text{DA}_3$) on $\text{Ag}:\text{CeO}_{2-x}(111)$. All distances are in Angstroms. The color code is the same as Figure S4. Reported energies include vdW corrections.

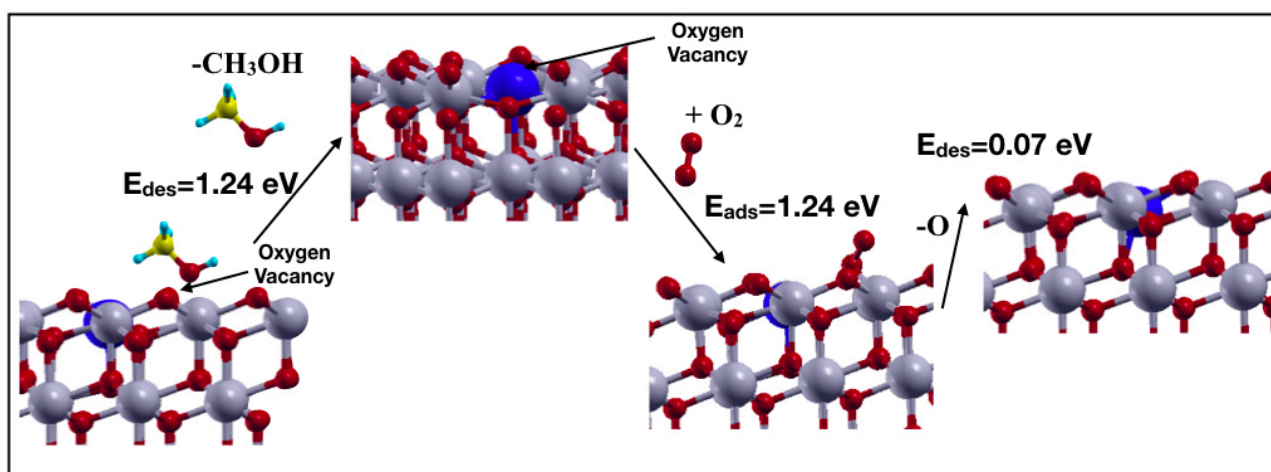


Figure S8 - Desorption of CH_3OH and adsorption of O_2 at the resulting surface oxygen vacancy on the $\text{Ag}:\text{CeO}_{2-x}(111)$ surface. The color code is the same as in Figure S4. Reported energies include vdW corrections.

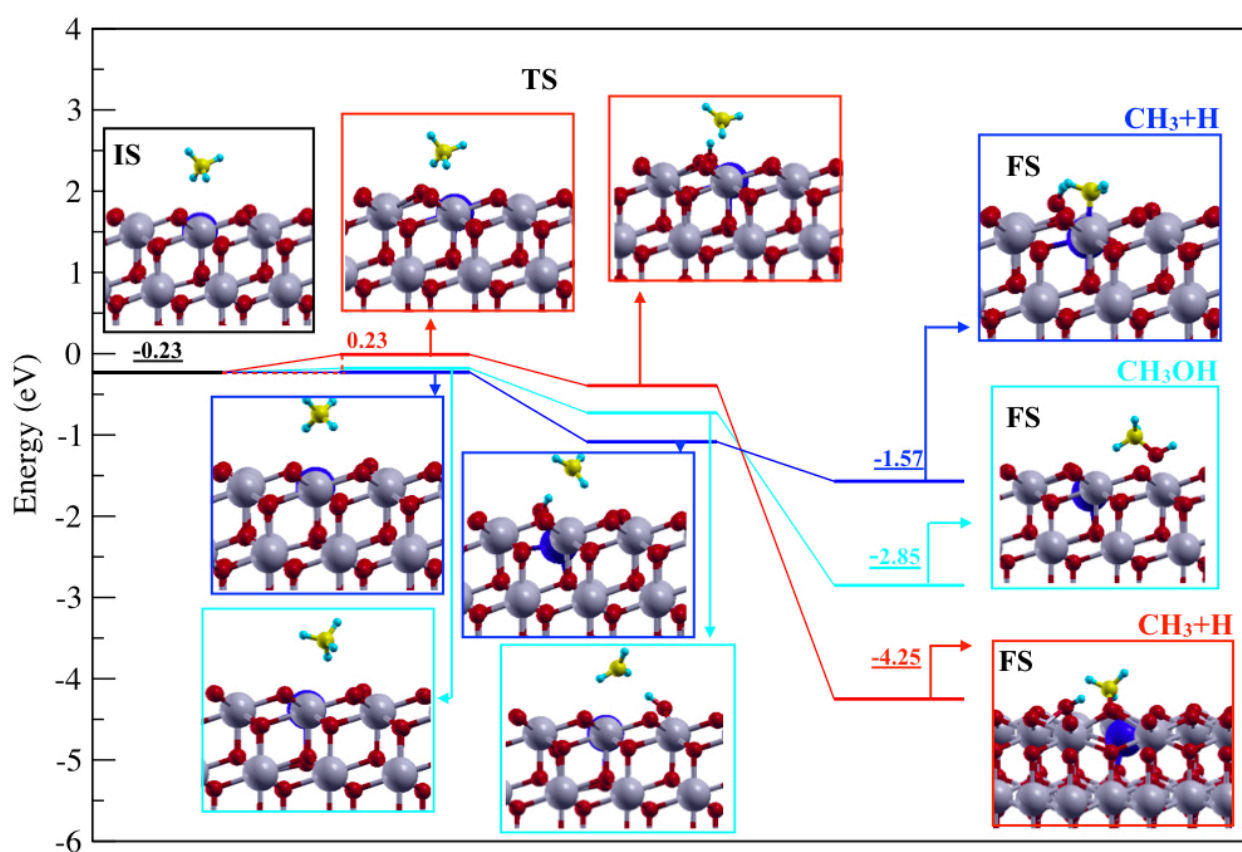


Figure S9 MEPs of the dissociative adsorption of CH_4 on the oxidized $\text{Ag}:\text{CeO}_2(111)$ surface: three different possible final states (FS) are considered. Reported energies include vdW corrections. The color code is the same as in Figure S4.

CH₄ on CeO₂(111)

C	5.8608016195	5.6264965571	10.2292818900
H	6.7605996207	6.1452578379	9.8603892161
H	5.8701117213	5.6218209443	11.3274882012
H	5.8540527124	4.5878865631	9.8609627794
H	4.9591016723	6.1510584163	9.8745678302
O	-0.0004432444	0.0010010798	7.7008095134
O	3.9029394160	0.0025127207	7.7016376201
O	7.8164999806	0.0015840503	7.7031244396
O	11.7167416501	0.0113102645	7.7034069058
O	-1.9547141801	3.3822801613	7.6998567735
O	1.9358651434	3.3773564851	7.6998609075
O	5.8623015173	3.3119545695	7.7137226602
O	9.7791104754	3.3745683438	7.7005719532
O	-3.9053632420	6.7618546402	7.7010125559
O	-0.0118758746	6.7528560419	7.7044824366
O	3.8478575368	6.7653283492	7.7469770242
O	7.8794602083	6.7925749323	7.7187639629
O	-5.8613197733	10.1477029440	7.7022157723
O	-1.9538501365	10.1449384697	7.6999014882
O	1.9121749273	10.1755836393	7.7236434906
O	5.9014608724	10.1857259077	7.7236995293
Ce	-0.0031875123	2.2541512647	6.9242862448
Ce	3.9010877087	2.2381248452	6.9240636395
Ce	7.8176107163	2.2413010965	6.9236920016
Ce	11.7189784913	2.2589901220	6.9285186869
Ce	-1.9562376714	5.6353671224	6.9243701369
Ce	1.9281823885	5.6297325256	6.9268932072
Ce	5.8648673765	5.6298480545	6.9659181862
Ce	9.7828535392	5.6399548672	6.9264566810
Ce	-3.9031471647	9.0199119709	6.9209691098
Ce	-0.0153468461	9.0237558870	6.9237612422
Ce	3.8970100872	9.0322504705	6.9496059255
Ce	7.8325491846	9.0352493085	6.9274490222
Ce	-5.8577316131	12.4058064953	6.9215002466
Ce	-1.9566377129	12.4004498315	6.9197406163
Ce	1.9438458213	12.4105602922	6.9260574314
Ce	5.8703777834	12.4112916633	6.9291620645
O	0.0128096136	-2.2456719833	6.1547799946
O	3.9045595011	-2.2548813061	6.1643367080
O	7.8016857951	-2.2490415614	6.1583273692
O	11.7150947875	-2.2403181112	6.1751768962
O	-1.9516990181	1.1284712144	6.1601943854
O	1.9509383000	1.1241696168	6.1601281756
O	5.8597148959	1.1075083731	6.1528995912
O	9.7651134968	1.1242745786	6.1586191294
O	-3.9015965218	4.5108576048	6.1577842588
O	-0.0087479905	4.5067269335	6.1573377447
O	3.9009123599	4.5037289036	6.1834147351

O	7.8199733291	4.5043870039	6.1817084238
O	-5.8415643084	7.9014284076	6.1521989748
O	-1.9553203438	7.8917415774	6.1615712917
O	1.9282969921	7.8947990119	6.1677331569
O	5.8684060225	7.8938078695	6.1939930649
O	0.0006217574	2.2542639425	4.6361855769
O	3.9063023644	2.2570372327	4.6428606676
O	7.8113215933	2.2575237130	4.6409201002
O	11.7172016826	2.2547257311	4.6384744951
O	-1.9533547109	5.6393482018	4.6350578178
O	1.9547071694	5.6363446700	4.6461012020
O	5.8589271477	5.6382087914	4.6314218048
O	9.7620924175	5.6366394500	4.6413736168
O	-3.8995131538	9.0249581524	4.6345753207
O	-0.0053122038	9.0240255608	4.6389569943
O	3.9073032808	9.0196196634	4.6252419739
O	7.8084678309	9.0192817740	4.6450371265
O	-5.8537572905	12.4049532368	4.6346326486
O	-1.9575439517	12.3966799706	4.6329808267
O	1.9525488751	12.4006163757	4.6402019044
O	5.8579352505	12.4007702228	4.6419827944
Ce	0.0006298078	-2.2542084210	3.8669850066
Ce	3.9057452840	-2.2549052565	3.8685801016
Ce	7.8101772935	-2.2546271860	3.8678948674
Ce	11.7184514294	-2.2591864018	3.8703133456
Ce	-1.9537691712	1.1272347822	3.8689788849
Ce	1.9522036556	1.1284248428	3.8677688377
Ce	5.8588026791	1.1255540147	3.8677316516
Ce	9.7661247728	1.1280141991	3.8672039855
Ce	-3.9062439146	4.5095759363	3.8673335054
Ce	-0.0015870366	4.5092932046	3.8665319838
Ce	3.9106565456	4.5123372691	3.8742252362
Ce	7.8079758155	4.5134198675	3.8730611231
Ce	-5.8578477801	7.8930476271	3.8675412346
Ce	-1.9529110853	7.8918331826	3.8679993285
Ce	1.9543280587	7.8959529792	3.8707248678
Ce	5.8556251950	7.8898823728	3.8753878093
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O	3.9063181642	0.0027115920	3.0852965771
O	7.8121435879	0.0004773062	3.0878180493
O	11.7177522816	-0.0019720335	3.0886585787
O	-1.9535677229	3.3820046871	3.0874255726
O	1.9560783038	3.3850188833	3.0886582855
O	5.8580280295	3.3811720096	3.0886334724
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O	0.0032179977	6.7660371131	3.0883338657
O	3.9033198605	6.7620497259	3.0891239531
O	7.8124040737	6.7675552247	3.0892860171
O	-5.8607211944	10.1468308605	3.0871740017
O	-1.9519745224	10.1474329240	3.0820838186

O	1.9499927639	10.1487959829	3.0875570544
O	5.8623211714	10.1477276669	3.0885014351
O	0.0000000000	-2.2550884807	1.5945886695
O	3.9059278863	-2.2550884807	1.5945886695
O	7.8118557727	-2.2550884807	1.5945886695
O	11.7177836590	-2.2550884807	1.5945886695
O	-1.9529639432	1.1275442326	1.5945886695
O	1.9529639432	1.1275442326	1.5945886695
O	5.8588918295	1.1275442326	1.5945886695
O	9.7648197159	1.1275442326	1.5945886695
O	-3.9059278863	4.5101769458	1.5945886695
O	0.0000000000	4.5101769458	1.5945886695
O	3.9059278863	4.5101769458	1.5945886695
O	7.8118557727	4.5101769458	1.5945886695
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O	-1.9529639432	5.6377214284	0.0000000000
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O	5.8588918295	5.6377214284	0.0000000000
O	9.7648197159	5.6377214284	0.0000000000
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O	7.8118557727	9.0203539073	0.0000000000
O	-5.8588918295	12.4029868549	0.0000000000
O	-1.9529639432	12.4029868549	0.0000000000
O	1.9529639432	12.4029868549	0.0000000000
O	5.8588918295	12.4029868549	0.0000000000

TS for the reaction $\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}$ on the $\text{CeO}_2(111)$ surface

C	6.1058858100	4.6262117727	10.1485409540
H	6.7333811406	5.5039819874	9.9771212281
H	5.0697447115	4.7322409054	10.4716603123
H	6.5449979081	3.6315803883	10.1157222188
H	3.7872235716	6.6549229381	9.1188074300
O	0.0016846391	0.0051701024	7.7081537720
O	3.8984891748	0.0065257136	7.7016603133
O	7.8185115326	-0.0024188084	7.7083732292
O	11.7109453451	0.0280397271	7.7186876347
O	-1.9639101628	3.3734120493	7.7086213068
O	1.9033665793	3.3731343368	7.7146611829
O	5.8505652484	3.2426625850	7.6816003961
O	9.7865767792	3.3493825321	7.7221251497
O	-3.8951778130	6.7602245711	7.7081166521
O	-0.0259189290	6.7232354814	7.7122214685
O	3.8112561968	6.7066743310	8.1329296463
O	7.9288865552	6.8029726707	7.7409245826
O	-5.8496590046	10.1478921987	7.7060252240
O	-1.9430789274	10.1353851404	7.7008695342
O	1.8696367903	10.1882360508	7.7141980821
O	5.9526578122	10.2168816961	7.7260305064
Ce	-0.0192575614	2.2351946772	6.9265654200
Ce	3.9002195371	2.2349730470	6.9212215573
Ce	7.8296691528	2.2213874221	6.9159400638
Ce	11.7116559430	2.2472414327	6.9380098668
Ce	-1.9767027763	5.6278924790	6.9263507260
Ce	1.8518063192	5.5744683398	6.9096725509
Ce	5.9329229797	5.5785125002	6.9671587366
Ce	9.7854014977	5.6401583272	6.9313914701
Ce	-3.8991806839	9.0202498617	6.9197286699
Ce	-0.0037782709	9.0207607951	6.9276043643
Ce	3.9044618443	9.1055915211	6.9509645275
Ce	7.8328935487	9.0263326798	6.9433506905
Ce	-5.8530609689	12.4007243804	6.9191061114
Ce	-1.9531140328	12.3950929139	6.9122265437
Ce	1.9428027549	12.4177810536	6.9244228342
Ce	5.8764226252	12.4152663372	6.9299742651
O	0.0341459339	-2.2399372543	6.1464845988
O	3.9114010137	-2.2561220248	6.1662622756
O	7.7899072194	-2.2451466014	6.1479300745
O	11.7187615802	-2.2014259829	6.1726485334
O	-1.9521196388	1.1221867166	6.1599149805
O	1.9488304406	1.1243421092	6.1590937030
O	5.8593019394	1.0789139294	6.1386574973
O	9.7618662387	1.1169163084	6.1510912441
O	-3.9097207274	4.5086091925	6.1615181431
O	-0.0364096028	4.4862558772	6.1515250558
O	3.8582590728	4.5735779312	6.2063433759
O	7.8614787084	4.4774343757	6.1780702185

O	-5.8264198857	7.9072238543	6.1472975806
O	-1.9499119635	7.8887816714	6.1612849635
O	1.9906524100	7.8151555693	6.2041077675
O	5.7956471941	7.8459888615	6.2487925559
O	-0.0045384301	2.2465983023	4.6337488149
O	3.9074219000	2.2754858191	4.6565603779
O	7.8120414809	2.2464267677	4.6319243429
O	11.7170757404	2.2524521368	4.6393374690
O	-1.9615419422	5.6352632417	4.6349264492
O	1.9190351261	5.6154113228	4.6282217961
O	5.8780630337	5.6233325139	4.6229357174
O	9.7667102413	5.6408152444	4.6376713117
O	-3.8927420206	9.0271288465	4.6328809884
O	0.0247993184	9.0073337885	4.6597323017
O	3.9082032230	9.0387953309	4.6198098762
O	7.7830637461	9.0002316006	4.6685900049
O	-5.8432077144	12.4060491500	4.6314439302
O	-1.9615797997	12.3874289707	4.6211419665
O	1.9491110660	12.3998602472	4.6334465727
O	5.8664679753	12.4010135075	4.6365262372
Ce	-0.0002124221	-2.2583781148	3.8688040349
Ce	3.9079975915	-2.2573327611	3.8663342622
Ce	7.8145252203	-2.2578632944	3.8649685096
Ce	11.7204281414	-2.2535607373	3.8673952557
Ce	-1.9557451535	1.1232485783	3.8676864092
Ce	1.9502114306	1.1280398222	3.8660418409
Ce	5.8600624117	1.1232587923	3.8635002767
Ce	9.7674897562	1.1244964143	3.8627298754
Ce	-3.9107044573	4.5069666690	3.8681658791
Ce	-0.0141847037	4.5000199699	3.8546882990
Ce	3.9087502364	4.5152386255	3.8853665212
Ce	7.8146905657	4.5077022254	3.8699469006
Ce	-5.8592437544	7.8902602849	3.8690320207
Ce	-1.9501568781	7.8878823589	3.8679360592
Ce	1.9608701761	7.8877913716	3.8836813020
Ce	5.8518107390	7.8829958388	3.8935259508
O	0.0025332998	-0.0027918637	3.0854667574
O	3.9053677202	0.0096046050	3.0858471661
O	7.8118890839	-0.0030468560	3.0835062951
O	11.7188924826	-0.0009001353	3.0853969897
O	-1.9580283840	3.3789407929	3.0833787073
O	1.9545204813	3.3767249491	3.0856750212
O	5.8561294546	3.3763752637	3.0864264082
O	9.7656373145	3.3814519437	3.0858822922
O	-3.9061401820	6.7665435126	3.0861186411
O	-0.0030751340	6.7675766833	3.0859320413
O	3.9011233005	6.7597976645	3.1020968795
O	7.8147152009	6.7700307167	3.0873967318
O	-5.8674418410	10.1406722305	3.0932418305
O	-1.9419646684	10.1372268864	3.0855635282
O	1.9487565322	10.1451861886	3.0854264247

O	5.8669265210	10.1453796269	3.0870270392
O	0.0000000000	-2.2550884807	1.5945886695
O	3.9059278863	-2.2550884807	1.5945886695
O	7.8118557727	-2.2550884807	1.5945886695
O	11.7177836590	-2.2550884807	1.5945886695
O	-1.9529639432	1.1275442326	1.5945886695
O	1.9529639432	1.1275442326	1.5945886695
O	5.8588918295	1.1275442326	1.5945886695
O	9.7648197159	1.1275442326	1.5945886695
O	-3.9059278863	4.5101769458	1.5945886695
O	0.0000000000	4.5101769458	1.5945886695
O	3.9059278863	4.5101769458	1.5945886695
O	7.8118557727	4.5101769458	1.5945886695
O	-5.8588918295	7.8928098935	1.5945886695
O	-1.9529639432	7.8928098935	1.5945886695
O	1.9529639432	7.8928098935	1.5945886695
O	5.8588918295	7.8928098935	1.5945886695
Ce	0.0000000000	0.0000000000	0.7972944519
Ce	3.9059278863	0.0000000000	0.7972944519
Ce	7.8118557727	0.0000000000	0.7972944519
Ce	11.7177836590	0.0000000000	0.7972944519
Ce	-1.9529639432	3.3826327133	0.7972944519
Ce	1.9529639432	3.3826327133	0.7972944519
Ce	5.8588918295	3.3826327133	0.7972944519
Ce	9.7648197159	3.3826327133	0.7972944519
Ce	-3.9059278863	6.7652654266	0.7972944519
Ce	0.0000000000	6.7652654266	0.7972944519
Ce	3.9059278863	6.7652654266	0.7972944519
Ce	7.8118557727	6.7652654266	0.7972944519
Ce	-5.8588918295	10.1478979055	0.7972944519
Ce	-1.9529639432	10.1478979055	0.7972944519
Ce	1.9529639432	10.1478979055	0.7972944519
Ce	5.8588918295	10.1478979055	0.7972944519
O	0.0000000000	2.2550884807	0.0000000000
O	3.9059278863	2.2550884807	0.0000000000
O	7.8118557727	2.2550884807	0.0000000000
O	11.7177836590	2.2550884807	0.0000000000
O	-1.9529639432	5.6377214284	0.0000000000
O	1.9529639432	5.6377214284	0.0000000000
O	5.8588918295	5.6377214284	0.0000000000
O	9.7648197159	5.6377214284	0.0000000000
O	-3.9059278863	9.0203539073	0.0000000000
O	0.0000000000	9.0203539073	0.0000000000
O	3.9059278863	9.0203539073	0.0000000000
O	7.8118557727	9.0203539073	0.0000000000
O	-5.8588918295	12.4029868549	0.0000000000
O	-1.9529639432	12.4029868549	0.0000000000
O	1.9529639432	12.4029868549	0.0000000000
O	5.8588918295	12.4029868549	0.0000000000

CH₃+H on CeO₂(111)

C	5.8930507685	3.1502306695	9.4920326820
H	6.1655189022	4.1085456615	9.9787504681
H	4.9078608609	2.8383009049	9.8958150187
H	6.6319579029	2.3890436773	9.8188140808
H	3.7238164328	6.6755073004	9.1481623135
O	0.0038041608	0.0079890767	7.7156105997
O	3.8947888023	0.0361746281	7.7021164364
O	7.8039136443	0.0226867265	7.7099363005
O	11.7129165416	0.0325743679	7.7328706683
O	-1.9641387578	3.3621117181	7.7163511673
O	1.8948334995	3.3451842854	7.7304573946
O	5.8620417061	3.2757662830	8.0710125344
O	9.7845560548	3.3233901079	7.7297506886
O	-3.8884861180	6.7623204651	7.7100095838
O	-0.0303675938	6.6976325826	7.7239595349
O	3.7883470002	6.6758331932	8.1633829561
O	8.0027291339	6.8181720829	7.7542594010
O	-5.8310165951	10.1722567846	7.7075607203
O	-1.9556357009	10.1736206134	7.7011976671
O	1.7906955175	10.2259382824	7.7311173755
O	5.9933358795	10.2576467082	7.7518581307
Ce	-0.0414756007	2.2288739293	6.9283786858
Ce	3.8078761896	2.2173226693	6.9043249581
Ce	7.9089748900	2.2053696027	6.9070181356
Ce	11.7285682775	2.2374392076	6.9412135365
Ce	-1.9779358417	5.6347483597	6.9299848239
Ce	1.8398149900	5.5766660494	6.9137067694
Ce	5.9333625970	5.6721185980	6.9477150563
Ce	9.7862456020	5.6604216797	6.9421017637
Ce	-3.8895296279	9.0372044915	6.9177413625
Ce	-0.0018631393	9.0419686399	6.9320274502
Ce	3.9142809909	9.1030719209	6.9651764397
Ce	7.8464162179	9.0445725783	6.9343236327
Ce	-5.8652257526	12.3930031962	6.9166007247
Ce	-1.9554294151	12.4224463202	6.9164117632
Ce	1.9483720318	12.3999897197	6.9277188566
Ce	5.8774592253	12.4042729805	6.9405515422
O	0.0449808368	-2.2313086656	6.1399701734
O	3.9144134920	-2.2321912734	6.1636557544
O	7.7676887488	-2.2163328134	6.1363570788
O	11.7140085902	-2.1960149586	6.1804649229
O	-1.9545580678	1.1184330351	6.1601997912
O	1.9271023961	1.1188460139	6.1551199169
O	5.8519249334	1.2301440906	6.1887436977
O	9.7797164096	1.1041196301	6.1505940484
O	-3.9103927928	4.5054274342	6.1682341102
O	-0.0370843828	4.4784580056	6.1536668933
O	3.8820802428	4.4908777022	6.2274344224
O	7.8015755847	4.4241389237	6.2075297559

O	-5.8027316674	7.9251360074	6.1392806713
O	-1.9449298049	7.8998224166	6.1692847559
O	1.9730934510	7.7999989445	6.2117633552
O	5.8902642903	7.9050987455	6.1983713825
O	-0.0122021575	2.2443153252	4.6312277789
O	3.8769337181	2.2532108815	4.6428322694
O	7.8386589149	2.2328996779	4.6259958635
O	11.7195210419	2.2513593383	4.6391922610
O	-1.9617305697	5.6412928857	4.6405062847
O	1.9327088192	5.6023631778	4.6422966412
O	5.8661617604	5.6291257245	4.6060081797
O	9.7459243329	5.6327982717	4.6588711946
O	-3.8788765843	9.0420105598	4.6311699210
O	0.0238185836	9.0194705193	4.6609157910
O	3.8958403836	9.0358996692	4.6111585584
O	7.8218798245	9.0259814401	4.6418603777
O	-5.8432020179	12.4111679233	4.6260749226
O	-1.9683607873	12.4499808977	4.6473293840
O	1.9512724838	12.3980808215	4.6317071214
O	5.8660265385	12.3992806134	4.6376787370
Ce	0.0015886246	-2.2571032551	3.8636336303
Ce	3.9088112007	-2.2449546786	3.8644692768
Ce	7.8152513888	-2.2481409191	3.8635307621
Ce	11.7205391450	-2.2593827935	3.8712225030
Ce	-1.9583294085	1.1187351094	3.8664225884
Ce	1.9378162204	1.1240575619	3.8527673044
Ce	5.8588219580	1.1412333580	3.8726062545
Ce	9.7773635401	1.1183520392	3.8541295894
Ce	-3.9133512643	4.5075507491	3.8734412397
Ce	-0.0159709835	4.4990889123	3.8555923577
Ce	3.9062720253	4.5153701515	3.8887112532
Ce	7.8113122655	4.5095297833	3.8761357566
Ce	-5.8546439607	7.8979524417	3.8675296561
Ce	-1.9456143401	7.8945911143	3.8720370681
Ce	1.9640287943	7.8903134693	3.8886857969
Ce	5.8588277141	7.8976027254	3.8876985907
O	-0.0018660553	-0.0025744212	3.0809341436
O	3.9066126104	0.0103383458	3.0797590345
O	7.8100666805	-0.0018027494	3.0816915788
O	11.7210135828	-0.0025795706	3.0833046922
O	-1.9605057181	3.3826775577	3.0852922268
O	1.9471328849	3.3786712494	3.0824813787
O	5.8567168747	3.3716770935	3.0959483475
O	9.7680227919	3.3859114267	3.0864292599
O	-3.9085111454	6.7655303254	3.0934025609
O	-0.0002979384	6.7663122978	3.0923751656
O	3.8941578017	6.7571231174	3.0993182723
O	7.8210207332	6.7673024447	3.0882708161
O	-5.8513940663	10.1494533669	3.0849740472
O	-1.9399663587	10.1579247208	3.0925103778
O	1.9437062834	10.1491470006	3.0828655690

O	5.8659700219	10.1499617320	3.0858204472
O	0.0000000000	-2.2550884807	1.5945886695
O	3.9059278863	-2.2550884807	1.5945886695
O	7.8118557727	-2.2550884807	1.5945886695
O	11.7177836590	-2.2550884807	1.5945886695
O	-1.9529639432	1.1275442326	1.5945886695
O	1.9529639432	1.1275442326	1.5945886695
O	5.8588918295	1.1275442326	1.5945886695
O	9.7648197159	1.1275442326	1.5945886695
O	-3.9059278863	4.5101769458	1.5945886695
O	0.0000000000	4.5101769458	1.5945886695
O	3.9059278863	4.5101769458	1.5945886695
O	7.8118557727	4.5101769458	1.5945886695
O	-5.8588918295	7.8928098935	1.5945886695
O	-1.9529639432	7.8928098935	1.5945886695
O	1.9529639432	7.8928098935	1.5945886695
O	5.8588918295	7.8928098935	1.5945886695
Ce	0.0000000000	0.0000000000	0.7972944519
Ce	3.9059278863	0.0000000000	0.7972944519
Ce	7.8118557727	0.0000000000	0.7972944519
Ce	11.7177836590	0.0000000000	0.7972944519
Ce	-1.9529639432	3.3826327133	0.7972944519
Ce	1.9529639432	3.3826327133	0.7972944519
Ce	5.8588918295	3.3826327133	0.7972944519
Ce	9.7648197159	3.3826327133	0.7972944519
Ce	-3.9059278863	6.7652654266	0.7972944519
Ce	0.0000000000	6.7652654266	0.7972944519
Ce	3.9059278863	6.7652654266	0.7972944519
Ce	7.8118557727	6.7652654266	0.7972944519
Ce	-5.8588918295	10.1478979055	0.7972944519
Ce	-1.9529639432	10.1478979055	0.7972944519
Ce	1.9529639432	10.1478979055	0.7972944519
Ce	5.8588918295	10.1478979055	0.7972944519
O	0.0000000000	2.2550884807	0.0000000000
O	3.9059278863	2.2550884807	0.0000000000
O	7.8118557727	2.2550884807	0.0000000000
O	11.7177836590	2.2550884807	0.0000000000
O	-1.9529639432	5.6377214284	0.0000000000
O	1.9529639432	5.6377214284	0.0000000000
O	5.8588918295	5.6377214284	0.0000000000
O	9.7648197159	5.6377214284	0.0000000000
O	-3.9059278863	9.0203539073	0.0000000000
O	0.0000000000	9.0203539073	0.0000000000
O	3.9059278863	9.0203539073	0.0000000000
O	7.8118557727	9.0203539073	0.0000000000
O	-5.8588918295	12.4029868549	0.0000000000
O	-1.9529639432	12.4029868549	0.0000000000
O	1.9529639432	12.4029868549	0.0000000000
O	5.8588918295	12.4029868549	0.0000000000

CH₄ on Ag:CeO_{2-x} (111)

C	1.8130318237	3.2561413182	9.1681115922
H	2.4923319122	3.6386943290	9.9403756179
H	1.9529991771	2.1660253771	9.0584862937
H	2.0115589427	3.7946671327	8.2242280178
H	0.7764625214	3.4675455914	9.4764215669
O	-0.0126532799	-0.0013373561	7.6825038134
O	3.9196384661	0.0046084244	7.7062400437
O	7.7757409147	0.0019790160	7.7387275040
O	11.7694881932	0.0030244980	7.7353658666
O	-2.0328204873	3.2756166664	7.7737528580
O	5.9554272169	3.3157888557	7.7245618402
O	9.7705529435	3.3708343877	7.7178699986
O	-3.9521956379	6.7820804467	7.6982081654
O	-0.4053019103	6.9751962764	7.8446645475
O	4.1476857260	6.8642664203	7.8030819331
O	7.8290686539	6.7516666579	7.7204763766
O	-5.8744697389	10.2027192516	7.7093323269
O	-2.0058298455	10.1712982688	7.7203042442
O	2.0178486786	10.2014017054	7.7688273876
O	5.8805514559	10.1725896921	7.7190376493
Ce	-0.1879005107	2.2188982347	6.8669890178
Ce	4.0884591996	2.1621014984	6.8848938677
Ce	7.8580088238	2.2431079382	6.9401092040
Ce	11.6898655024	2.2555816181	6.9435480051
Ce	-1.9484060336	5.6794861613	6.9526087496
Ag	2.4726559452	5.9648202860	6.6849875677
Ce	5.9491695342	5.6544523884	6.9587840902
Ce	9.7921522280	5.6493528753	6.9247880360
Ce	-3.9280743958	9.0377399949	6.9133316264
Ce	-0.0630103502	8.9883896271	6.9605607370
Ce	3.9459118332	9.0761084774	6.9484326038
Ce	7.8228485005	9.0443568405	6.9123276833
Ce	-5.8671897466	12.4194218375	6.9420754667
Ce	-1.9281510916	12.3591130193	6.9286888332
Ce	1.9583599338	12.3871874025	6.9645125605
Ce	5.8483673308	12.3934744318	6.9222069733
O	0.0056490282	-2.2455063410	6.1534130864
O	3.8867560023	-2.2352476573	6.1573278123
O	7.7952127949	-2.2833738575	6.1817188283
O	11.7509637291	-2.2555034029	6.1569138008
O	-1.9922848626	1.1085605413	6.1295360592
O	1.9616449080	1.3845447744	6.3008314560
O	5.9043542182	1.0899119341	6.1413260122
O	9.7683698701	1.1100203142	6.1795324257
O	-3.9018525556	4.5100124780	6.1684307567
O	-0.0373600709	4.3722568555	6.2367682632
O	3.8428182306	4.3505447918	6.3110214201
O	7.8448852796	4.5144596933	6.1604298555
O	-5.8781622358	7.9186280376	6.1654044671

O	-2.0510409411	7.9525845503	6.0969488622
O	1.9246504856	7.9778844183	6.2278069771
O	5.9257023886	7.9252381656	6.1441479275
O	-0.0319214165	2.2047386781	4.6018418888
O	3.9625672431	2.2194518235	4.6201427529
O	7.8294120139	2.2511098637	4.6397596629
O	11.6983590434	2.2524233775	4.6367669972
O	-1.9297713664	5.6428984727	4.6569253442
O	1.9475292242	5.6303628469	4.5470449042
O	5.8185614854	5.6048687402	4.6968237878
O	9.7742019368	5.6535636857	4.6394040348
O	-3.9561522459	9.0529476044	4.6131562288
O	-0.0038303445	9.0128450982	4.6406847753
O	3.9057149385	9.0153025146	4.6551079086
O	7.8274368367	9.0424745517	4.6193611901
O	-5.8636398947	12.5022726669	4.6981430096
O	-1.9427127823	12.3888791247	4.6360999086
O	1.9517774318	12.3905560168	4.6219820326
O	5.8559896031	12.4006104119	4.6261805085
Ce	-0.0055655384	-2.2400112453	3.8628712210
Ce	3.9050225041	-2.2412912756	3.8668511232
Ce	7.8199206870	-2.2739212888	3.8770000801
Ce	11.7111011431	-2.2622103870	3.8641862682
Ce	-1.9788146085	1.1187342690	3.8364905283
Ce	1.9530521021	1.1547927547	3.8868660754
Ce	5.8913861270	1.1077806489	3.8416755821
Ce	9.7682043405	1.1180681812	3.8688212750
Ce	-3.8943163488	4.5114556228	3.8756164873
Ce	0.0109964341	4.5231733961	3.9167845894
Ce	3.9034236691	4.5017609093	3.8815477506
Ce	7.8201948319	4.5050162988	3.8707469872
Ce	-5.8633657175	7.9026554130	3.8659614389
Ce	-1.9632087139	7.8995960165	3.8581153302
Ce	1.9414396759	7.8934159863	3.8741333342
Ce	5.8551231426	7.8939789996	3.8716264406
O	0.0051300663	-0.0093153520	3.0748105053
O	3.9051901672	-0.0047974177	3.0829509577
O	7.8175387813	-0.0053735181	3.0817246692
O	11.7113291997	-0.0043865552	3.0790532416
O	-1.9619416729	3.3851353276	3.0907827061
O	1.9669562529	3.3588608514	3.1015459307
O	5.8694710547	3.3876635982	3.0859510440
O	9.7635653631	3.3877868580	3.0871038143
O	-3.9065720101	6.7646637976	3.0875791962
O	-0.0110079016	6.7749967713	3.0794130389
O	3.9276490736	6.7646471611	3.0874242253
O	7.7944766740	6.7542144068	3.1001847783
O	-5.8669909689	10.1956900249	3.0891216196
O	-1.9578323373	10.1537176636	3.0849087029
O	1.9554759923	10.1382448586	3.0853775832
O	5.8549453621	10.1463383277	3.0866480705

O	0.0000000000	-2.2550884807	1.5945886695
O	3.9059278863	-2.2550884807	1.5945886695
O	7.8118557727	-2.2550884807	1.5945886695
O	11.7177836590	-2.2550884807	1.5945886695
O	-1.9529639432	1.1275442326	1.5945886695
O	1.9529639432	1.1275442326	1.5945886695
O	5.8588918295	1.1275442326	1.5945886695
O	9.7648197159	1.1275442326	1.5945886695
O	-3.9059278863	4.5101769458	1.5945886695
O	0.0000000000	4.5101769458	1.5945886695
O	3.9059278863	4.5101769458	1.5945886695
O	7.8118557727	4.5101769458	1.5945886695
O	-5.8588918295	7.8928098935	1.5945886695
O	-1.9529639432	7.8928098935	1.5945886695
O	1.9529639432	7.8928098935	1.5945886695
O	5.8588918295	7.8928098935	1.5945886695
Ce	0.0000000000	0.0000000000	0.7972944519
Ce	3.9059278863	0.0000000000	0.7972944519
Ce	7.8118557727	0.0000000000	0.7972944519
Ce	11.7177836590	0.0000000000	0.7972944519
Ce	-1.9529639432	3.3826327133	0.7972944519
Ce	1.9529639432	3.3826327133	0.7972944519
Ce	5.8588918295	3.3826327133	0.7972944519
Ce	9.7648197159	3.3826327133	0.7972944519
Ce	-3.9059278863	6.7652654266	0.7972944519
Ce	0.0000000000	6.7652654266	0.7972944519
Ce	3.9059278863	6.7652654266	0.7972944519
Ce	7.8118557727	6.7652654266	0.7972944519
Ce	-5.8588918295	10.1478979055	0.7972944519
Ce	-1.9529639432	10.1478979055	0.7972944519
Ce	1.9529639432	10.1478979055	0.7972944519
Ce	5.8588918295	10.1478979055	0.7972944519
O	0.0000000000	2.2550884807	0.0000000000
O	3.9059278863	2.2550884807	0.0000000000
O	7.8118557727	2.2550884807	0.0000000000
O	11.7177836590	2.2550884807	0.0000000000
O	-1.9529639432	5.6377214284	0.0000000000
O	1.9529639432	5.6377214284	0.0000000000
O	5.8588918295	5.6377214284	0.0000000000
O	9.7648197159	5.6377214284	0.0000000000
O	-3.9059278863	9.0203539073	0.0000000000
O	0.0000000000	9.0203539073	0.0000000000
O	3.9059278863	9.0203539073	0.0000000000
O	7.8118557727	9.0203539073	0.0000000000
O	-5.8588918295	12.4029868549	0.0000000000
O	-1.9529639432	12.4029868549	0.0000000000
O	1.9529639432	12.4029868549	0.0000000000
O	5.8588918295	12.4029868549	0.0000000000

CH₃ +H on Ag:CeO_{2-x} (111)

C	4.4116059447	6.9319665910	9.5859751359
H	4.7318386155	7.9127357052	9.9941841273
H	3.4353899154	6.6650867198	10.0335430599
H	5.1569819795	6.1847044111	9.9339580302
H	2.0156449739	10.0609614405	9.1761109396
O	-0.0095291547	-0.0092150553	7.6743037452
O	3.9159027577	0.0051512708	7.6733784673
O	7.6719311372	0.0467756759	7.7392343560
O	11.8660837855	0.0432264323	7.7444014956
O	-2.0307375465	3.3267133322	7.7539296213
O	5.9525439395	3.3492483778	7.7516546533
O	9.7727830978	3.4051628582	7.7460586278
O	-3.9485865303	6.7599294760	7.7122479870
O	-0.3001255532	6.8916898962	7.7794932116
O	4.3359824526	6.9608488449	8.1661814615
O	7.8130029218	6.7406604750	7.7044123057
O	-5.8837169330	10.1876351509	7.7169165651
O	-2.0196531150	10.1380890999	7.7280050983
O	2.0061959077	10.1202077716	8.1910350685
O	5.8969524844	10.1153258963	7.7223742005
Ce	-0.1814309576	2.2164449990	6.8601242541
Ce	4.0861677984	2.2143345338	6.8622462075
Ce	7.8543341415	2.2475958701	6.9396075420
Ce	11.6958102041	2.2660431282	6.9424816399
Ce	-1.9793446683	5.6470357972	6.9462081182
Ag	1.8477154958	5.7838348981	6.8523614721
Ce	5.9463314687	5.5849457614	6.9251420559
Ce	9.7848866809	5.6353123376	6.9294966199
Ce	-3.9378717164	9.0320706014	6.9182744090
Ce	-0.1133952524	8.9478335698	6.9307564492
Ce	4.0006804182	9.0430145541	6.8977831278
Ce	7.8208458218	9.0197407047	6.9166277411
Ce	-5.8645611218	12.4119663523	6.9493230822
Ce	-1.9345968720	12.3740122006	6.9339527486
Ce	1.9497876890	12.4541841703	6.9777250775
Ce	5.8423400848	12.4018674628	6.9277920247
O	0.0022335694	-2.2587242570	6.1556291745
O	3.8796845647	-2.2509541382	6.1581599570
O	7.8228147267	-2.3580240557	6.2099584829
O	11.7135561376	-2.3297525678	6.1991439396
O	-1.9726406701	1.1286975236	6.1183134431
O	1.9576855282	1.4542437936	6.3462120088
O	5.8792917223	1.1360583391	6.1235220045
O	9.7721496879	1.1783390871	6.1863733258
O	-3.9142617192	4.5079049302	6.1597536036
O	-0.0058652590	4.3682567799	6.2427469833
O	3.9022818911	4.4423435963	6.3006710263
O	7.8420538172	4.4939436246	6.1578213967

O	-5.8745096237	7.9098815433	6.1707419358
O	-2.0556585904	7.9185771163	6.1188009092
O	2.0217486185	8.1599963427	6.2337982194
O	5.8544577557	7.8514240991	6.1465904490
O	-0.0268616885	2.2080856987	4.5983830240
O	3.9379411248	2.2378544198	4.6183312652
O	7.8284690259	2.2487844393	4.6304586207
O	11.7083609054	2.2557535499	4.6293763272
O	-1.9298233808	5.6228622027	4.6659887408
O	1.9587528335	5.6524576174	4.4597872825
O	5.8566075899	5.5968476706	4.6646880303
O	9.7689858430	5.6494863018	4.6406841307
O	-3.9498943478	9.0417675515	4.6171550671
O	-0.0281853611	8.9726246521	4.6351775150
O	3.9591119478	9.0207961891	4.6033166661
O	7.8113390816	9.0200033652	4.6406069489
O	-5.8650125109	12.5175776719	4.7140138201
O	-1.9290845579	12.3869435198	4.6569386356
O	1.9508787274	12.4116000658	4.6132065166
O	5.8332140170	12.3952329359	4.6478076514
Ce	-0.0111138341	-2.2426148471	3.8682849376
Ce	3.9084720326	-2.2434049271	3.8704945769
Ce	7.8255433820	-2.2797114984	3.8881049415
Ce	11.7049158801	-2.2623823687	3.8705537100
Ce	-1.9793226899	1.1210363688	3.8333600708
Ce	1.9518474431	1.1610771320	3.8842380075
Ce	5.8896683370	1.1171230424	3.8371549286
Ce	9.7672332246	1.1224385917	3.8687724597
Ce	-3.8979414655	4.5048221843	3.8681346964
Ce	0.0207346422	4.5288921884	3.8958375239
Ce	3.8811229450	4.5324708603	3.9035385009
Ce	7.8204949708	4.4956796844	3.8587904165
Ce	-5.8623202182	7.8951978994	3.8673174782
Ce	-1.9685553945	7.8875720238	3.8519569557
Ce	1.9562275874	7.8785575389	3.8980630993
Ce	5.8685579802	7.8837400077	3.8541553725
O	0.0004138394	-0.0157650520	3.0807020934
O	3.9064189692	-0.0078788608	3.0895884614
O	7.8109579495	-0.0075689267	3.0802912985
O	11.7158452898	-0.0024965635	3.0768756940
O	-1.9585894723	3.3859604148	3.0843741956
O	1.9562396687	3.3479528238	3.0956448670
O	5.8688500766	3.3793974208	3.0827915211
O	9.7675932080	3.3878453694	3.0824634451
O	-3.9077945532	6.7581404083	3.0885698607
O	-0.0357481764	6.7714501759	3.0714610364
O	3.9490411592	6.7717603431	3.0811028578
O	7.8126936709	6.7560024513	3.0886216519
O	-5.8714477338	10.1956739860	3.1027219964
O	-1.9591866102	10.1554269466	3.0902788159
O	1.9491201875	10.1374310291	3.0985916146

O	5.8747850512	10.1606703831	3.0799970443
O	0.0000000000	-2.2550884807	1.5945886695
O	3.9059278863	-2.2550884807	1.5945886695
O	7.8118557727	-2.2550884807	1.5945886695
O	11.7177836590	-2.2550884807	1.5945886695
O	-1.9529639432	1.1275442326	1.5945886695
O	1.9529639432	1.1275442326	1.5945886695
O	5.8588918295	1.1275442326	1.5945886695
O	9.7648197159	1.1275442326	1.5945886695
O	-3.9059278863	4.5101769458	1.5945886695
O	0.0000000000	4.5101769458	1.5945886695
O	3.9059278863	4.5101769458	1.5945886695
O	7.8118557727	4.5101769458	1.5945886695
O	-5.8588918295	7.8928098935	1.5945886695
O	-1.9529639432	7.8928098935	1.5945886695
O	1.9529639432	7.8928098935	1.5945886695
O	5.8588918295	7.8928098935	1.5945886695
Ce	0.0000000000	0.0000000000	0.7972944519
Ce	3.9059278863	0.0000000000	0.7972944519
Ce	7.8118557727	0.0000000000	0.7972944519
Ce	11.7177836590	0.0000000000	0.7972944519
Ce	-1.9529639432	3.3826327133	0.7972944519
Ce	1.9529639432	3.3826327133	0.7972944519
Ce	5.8588918295	3.3826327133	0.7972944519
Ce	9.7648197159	3.3826327133	0.7972944519
Ce	-3.9059278863	6.7652654266	0.7972944519
Ce	0.0000000000	6.7652654266	0.7972944519
Ce	3.9059278863	6.7652654266	0.7972944519
Ce	7.8118557727	6.7652654266	0.7972944519
Ce	-5.8588918295	10.1478979055	0.7972944519
Ce	-1.9529639432	10.1478979055	0.7972944519
Ce	1.9529639432	10.1478979055	0.7972944519
Ce	5.8588918295	10.1478979055	0.7972944519
O	0.0000000000	2.2550884807	0.0000000000
O	3.9059278863	2.2550884807	0.0000000000
O	7.8118557727	2.2550884807	0.0000000000
O	11.7177836590	2.2550884807	0.0000000000
O	-1.9529639432	5.6377214284	0.0000000000
O	1.9529639432	5.6377214284	0.0000000000
O	5.8588918295	5.6377214284	0.0000000000
O	9.7648197159	5.6377214284	0.0000000000
O	-3.9059278863	9.0203539073	0.0000000000
O	0.0000000000	9.0203539073	0.0000000000
O	3.9059278863	9.0203539073	0.0000000000
O	7.8118557727	9.0203539073	0.0000000000
O	-5.8588918295	12.4029868549	0.0000000000
O	-1.9529639432	12.4029868549	0.0000000000
O	1.9529639432	12.4029868549	0.0000000000
O	5.8588918295	12.4029868549	0.0000000000

CH₃OH on Ag:CeO_{2-x}(111)

C	3.5988340958	6.9780161724	9.7663615048
H	3.2551002481	7.9149198061	10.2302910248
H	2.7503969917	6.4996767841	9.2515055386
H	4.0156337336	6.2982626846	10.5249888847
H	5.3445558145	7.7768749097	9.1063417727
O	0.0025024422	-0.0039174560	7.6781333623
O	3.9048417652	0.0193907330	7.6817682582
O	7.6865580410	0.0626073553	7.7491266599
O	11.8748145650	0.0585260829	7.7580360435
O	-2.0105900167	3.3217199986	7.7548228222
O	5.9720892313	3.3370075144	7.7521063649
O	9.7852928039	3.4126791824	7.7443256608
O	-3.9424697917	6.7714272448	7.7154591586
O	-0.3013357619	6.9127554444	7.8077100796
O	4.5833688000	7.2545130577	8.7305763238
O	7.7653465855	6.7562298801	7.7330802755
O	-5.8983339483	10.1976732865	7.7175227368
O	-2.0262668973	10.1540567252	7.7293996484
O	1.9735450631	10.0197619469	7.7831423621
O	5.8935985286	10.0754870349	7.7560682219
Ce	-0.1788270407	2.2238577576	6.8648533098
Ce	4.0894611856	2.1966899614	6.8758805965
Ce	7.8723003347	2.2205695015	6.9432163471
Ce	11.7032230600	2.2598194059	6.9460151157
Ce	-1.9487818776	5.6761330542	6.9511828117
Ag	1.9138561761	5.6131412670	6.8167391085
Ce	5.9951628195	5.5383663918	6.8902737874
Ce	9.8137515017	5.6378799298	6.9298912701
Ce	-3.9174753245	9.0371597001	6.9224025188
Ce	-0.0111751628	8.9698181107	6.9537029357
Ce	3.8434429795	9.1342075531	6.8677547314
Ce	7.7828218911	9.0252328843	6.9334731202
Ce	-5.8725510097	12.4000766833	6.9558728925
Ce	-1.9394274583	12.3624773297	6.9300884117
Ce	1.9349650226	12.4049371815	6.9936522051
Ce	5.8459489633	12.4137219426	6.9293629311
O	-0.0172113032	-2.2611593175	6.1589022399
O	3.8738766241	-2.2459663763	6.1596497640
O	7.7604943403	-2.3046806185	6.1808446139
O	11.7739359858	-2.2608065807	6.1685812804
O	-1.9650107364	1.1270113194	6.1198251199
O	1.9623464497	1.4723763606	6.3463340605
O	5.8782654956	1.1261128184	6.1263698441
O	9.7823313565	1.1743376832	6.1805963278
O	-3.8998268654	4.5200108849	6.1656512942
O	0.0054295416	4.3844633838	6.2449598565
O	3.9226476565	4.4968546871	6.3853078819
O	7.8598951101	4.5017746634	6.1578958234
O	-5.8883902206	7.9042490412	6.1808802971

O	-2.0341469260	7.9316644698	6.1175836283
O	2.0793024656	7.8681233518	6.1931989008
O	5.7065451087	7.7753345011	6.2159716374
O	-0.0268722322	2.2163067110	4.6011471673
O	3.9453745232	2.2690160807	4.6408690354
O	7.8273897679	2.2500598201	4.6336820008
O	11.7172376034	2.2610614598	4.6317420765
O	-1.9192904552	5.6275287809	4.6670463771
O	1.9647855638	5.6109773656	4.3945724318
O	5.8693026601	5.5721295236	4.6513938126
O	9.7769987208	5.6485642343	4.6418748538
O	-3.9537464638	9.0432036318	4.6239470045
O	0.0268309486	8.9821475387	4.6637208878
O	3.9158086517	9.0631652880	4.5919356424
O	7.7580243180	8.9955521172	4.6753607207
O	-5.8729796444	12.5128066208	4.7170564374
O	-1.9583310741	12.3977245281	4.6363926406
O	1.9505941331	12.4042050478	4.6179746664
O	5.8543183645	12.4147318029	4.6266039372
Ce	-0.0198887724	-2.2418131467	3.8702055511
Ce	3.9037239100	-2.2426117051	3.8729635653
Ce	7.8250088392	-2.2748833265	3.8851824932
Ce	11.7048390025	-2.2392317397	3.8530523897
Ce	-1.9744008665	1.1248165487	3.8340047530
Ce	1.9506609525	1.1584675068	3.8856743991
Ce	5.8895925706	1.1154488603	3.8388900371
Ce	9.7700311861	1.1191859854	3.8752621119
Ce	-3.8875828161	4.5103548293	3.8728317885
Ce	0.0174718880	4.5234338793	3.8873217833
Ce	3.8844321701	4.5239714186	3.8887461818
Ce	7.8365312310	4.4895170900	3.8481032477
Ce	-5.8684723907	7.8945286041	3.8771022602
Ce	-1.9571245897	7.8967817666	3.8650213540
Ce	1.9525447278	7.8633646175	3.8849170258
Ce	5.8427326348	7.8852991133	3.8781087158
O	0.0094701584	-0.0108805934	3.0774925564
O	3.8956281616	0.0054515690	3.0922862710
O	7.8110676041	-0.0041577996	3.0822278639
O	11.7138334941	0.0060313935	3.0746522999
O	-1.9568295822	3.3892191762	3.0814857425
O	1.9622654477	3.3246641087	3.0833460618
O	5.8707221240	3.3747582520	3.0751956354
O	9.7719516173	3.3863292002	3.0833515361
O	-3.9044691506	6.7642761629	3.0938252430
O	-0.0391595133	6.7786753606	3.0722310036
O	3.9607849657	6.7730744674	3.0866356547
O	7.8063263864	6.7602798256	3.0955042951
O	-5.8878931019	10.1836240378	3.1142957038
O	-1.9541824587	10.1471295164	3.0971019687
O	1.9432655503	10.1479715048	3.0815655906
O	5.8735390238	10.1544261534	3.0816117269

O	0.0000000000	-2.2550884807	1.5945886695
O	3.9059278863	-2.2550884807	1.5945886695
O	7.8118557727	-2.2550884807	1.5945886695
O	11.7177836590	-2.2550884807	1.5945886695
O	-1.9529639432	1.1275442326	1.5945886695
O	1.9529639432	1.1275442326	1.5945886695
O	5.8588918295	1.1275442326	1.5945886695
O	9.7648197159	1.1275442326	1.5945886695
O	-3.9059278863	4.5101769458	1.5945886695
O	0.0000000000	4.5101769458	1.5945886695
O	3.9059278863	4.5101769458	1.5945886695
O	7.8118557727	4.5101769458	1.5945886695
O	-5.8588918295	7.8928098935	1.5945886695
O	-1.9529639432	7.8928098935	1.5945886695
O	1.9529639432	7.8928098935	1.5945886695
O	5.8588918295	7.8928098935	1.5945886695
Ce	0.0000000000	0.0000000000	0.7972944519
Ce	3.9059278863	0.0000000000	0.7972944519
Ce	7.8118557727	0.0000000000	0.7972944519
Ce	11.7177836590	0.0000000000	0.7972944519
Ce	-1.9529639432	3.3826327133	0.7972944519
Ce	1.9529639432	3.3826327133	0.7972944519
Ce	5.8588918295	3.3826327133	0.7972944519
Ce	9.7648197159	3.3826327133	0.7972944519
Ce	-3.9059278863	6.7652654266	0.7972944519
Ce	0.0000000000	6.7652654266	0.7972944519
Ce	3.9059278863	6.7652654266	0.7972944519
Ce	7.8118557727	6.7652654266	0.7972944519
Ce	-5.8588918295	10.1478979055	0.7972944519
Ce	-1.9529639432	10.1478979055	0.7972944519
Ce	1.9529639432	10.1478979055	0.7972944519
Ce	5.8588918295	10.1478979055	0.7972944519
O	0.0000000000	2.2550884807	0.0000000000
O	3.9059278863	2.2550884807	0.0000000000
O	7.8118557727	2.2550884807	0.0000000000
O	11.7177836590	2.2550884807	0.0000000000
O	-1.9529639432	5.6377214284	0.0000000000
O	1.9529639432	5.6377214284	0.0000000000
O	5.8588918295	5.6377214284	0.0000000000
O	9.7648197159	5.6377214284	0.0000000000
O	-3.9059278863	9.0203539073	0.0000000000
O	0.0000000000	9.0203539073	0.0000000000
O	3.9059278863	9.0203539073	0.0000000000
O	7.8118557727	9.0203539073	0.0000000000
O	-5.8588918295	12.4029868549	0.0000000000
O	-1.9529639432	12.4029868549	0.0000000000
O	1.9529639432	12.4029868549	0.0000000000
O	5.8588918295	12.4029868549	0.0000000000

CH₄ on CeO₂(100)

C	9.7648389018	5.8585400929	10.3230545232
H	10.5707782814	6.2688210079	10.9456087449
H	8.9592098403	5.4485555910	10.9462113359
H	10.1922778862	5.0588843201	9.6995515984
H	9.3370062624	6.6578812510	9.6993890337
O	-0.0066901983	1.9601945344	7.8659912926
O	3.9042193085	1.9488128168	7.8661775585
O	7.8077142705	1.9495803472	7.8693648425
O	11.7134596250	1.9715509572	7.8705332618
O	0.0147587048	5.8641456619	7.8716406549
O	3.8914581421	5.8539767349	7.8718110783
O	7.7676304980	5.8506458377	7.8484945012
O	11.7622710059	5.8676058921	7.8486698617
O	0.0012675673	9.7692255869	7.8659814184
O	3.9121474203	9.7578661331	7.8661940884
O	7.8157023149	9.7468678682	7.8702975313
O	11.7215014931	9.7683467688	7.8695716692
O	0.0012149936	13.6773174198	7.8656397747
O	3.9046186974	13.6644429347	7.8658540539
O	7.8116234481	13.6606300928	7.8665170774
O	11.7178801355	13.6810162398	7.8667126863
Ce	13.6705195117	13.6720394019	6.7907206086
Ce	9.7649573451	13.6707101209	6.7907534340
Ce	5.8589111092	13.6693939639	6.7907339043
Ce	1.9531103998	13.6707327597	6.7913292927
Ce	13.6704588292	9.7641802842	6.7909302632
Ce	9.7660835648	9.7658664577	6.7942552077
Ce	5.8605954390	9.7619116588	6.7912513148
Ce	1.9537979681	9.7644311073	6.7906438961
Ce	13.6845967257	5.8597502275	6.7868735821
Ce	9.7651308152	5.8588681127	6.8066083921
Ce	5.8451784761	5.8580101679	6.7868884402
Ce	1.9532287495	5.8588697688	6.7940434595
Ce	13.6687563758	1.9561228858	6.7912450809
Ce	9.7637865823	1.9521632905	6.7942443961
Ce	5.8589312013	1.9538046395	6.7909226388
Ce	1.9523561652	1.9535702994	6.7906535360
O	1.9532200314	-0.0004348548	5.6251535898
O	5.8606740263	0.0009969803	5.6263876130
O	9.7645442855	-0.0012299923	5.6259609451
O	13.6686790384	0.0018992340	5.6263284460
O	0.0007794513	1.9513683560	5.2977214518
O	3.9063320093	1.9522094429	5.2976925479
O	7.8166293634	1.9545800911	5.2984127073
O	11.7130323165	1.9527055895	5.2989053854
O	1.9532182503	3.9027955822	5.6233051641
O	5.8591985230	3.9041556263	5.6187962235
O	9.7644428719	3.9113035993	5.6444492485

O	13.6700933281	3.9041911858	5.6186165508
O	-0.0001121001	5.8582992378	5.2961618304
O	3.9062162844	5.8594753283	5.2962101858
O	7.8293166609	5.8599481955	5.2925818132
O	11.7005237387	5.8578518528	5.2926318090
O	1.9529858007	7.8150561181	5.6233747677
O	5.8595746951	7.8136719510	5.6187143708
O	9.7654779272	7.8065402736	5.6445806127
O	13.6704754059	7.8136895746	5.6188574996
O	-0.0002294186	9.7656413200	5.2976352089
O	3.9053261079	9.7664846879	5.2977748693
O	7.8167938498	9.7651347055	5.2988394377
O	11.7131714457	9.7632840613	5.2984818579
O	1.9529186657	11.7182863363	5.6250626129
O	5.8609071008	11.7159563097	5.6262022846
O	9.7653198777	11.7190815051	5.6258540789
O	13.6689148940	11.7168327375	5.6263121818
O	-0.0026249398	13.6704522203	5.2970635686
O	3.9086399908	13.6710616232	5.2971278758
O	7.8116504928	13.6714256713	5.2971319379
O	11.7181124444	13.6700757982	5.2971905737
Ce	11.7175445850	11.7170389548	4.0974842297
Ce	7.8123067511	11.7174149707	4.0975685509
Ce	3.9061557426	11.7175964557	4.0971710524
Ce	-0.0001491908	11.7175210088	4.0972201734
Ce	11.7172836065	7.8096003806	4.0988362745
Ce	7.8126013206	7.8101296338	4.0989314541
Ce	3.9055281693	7.8128797664	4.0962706423
Ce	0.0004641336	7.8126709711	4.0963222006
Ce	11.7170780141	3.9077107549	4.0988265097
Ce	7.8123961188	3.9082588504	4.0988423677
Ce	3.9055043588	3.9051265618	4.0962535500
Ce	0.0004373389	3.9049073455	4.0962718141
Ce	11.7173663497	0.0004014356	4.0975503024
Ce	7.8121351090	0.0007818730	4.0975780814
Ce	3.9061202611	0.0002723213	4.0972156894
Ce	-0.0001888126	0.0001972337	4.0972701693
O	1.9529639432	0.0000000000	2.7619091062
O	5.8588918295	0.0000000000	2.7619091062
O	9.7648197159	0.0000000000	2.7619091062
O	13.6707476022	0.0000000000	2.7619091062
O	0.0000000000	1.9529639432	2.7619091062
O	3.9059278863	1.9529639432	2.7619091062
O	7.8118557727	1.9529639432	2.7619091062
O	11.7177836590	1.9529639432	2.7619091062
O	1.9529639432	3.9059278863	2.7619091062
O	5.8588918295	3.9059278863	2.7619091062
O	9.7648197159	3.9059278863	2.7619091062
O	13.6707476022	3.9059278863	2.7619081687
O	0.0000000000	5.8588918295	2.7619091062
O	3.9059278863	5.8588918295	2.7619091062

O	7.8118557727	5.8588918295	2.7619091062
O	11.7177836590	5.8588918295	2.7619091062
O	1.9529639432	7.8118557727	2.7619091062
O	5.8588918295	7.8118557727	2.7619091062
O	9.7648197159	7.8118557727	2.7619091062
O	13.6707476022	7.8118557727	2.7619091062
O	0.0000000000	9.7648197159	2.7619091062
O	3.9059278863	9.7648197159	2.7619091062
O	7.8118557727	9.7648197159	2.7619091062
O	11.7177836590	9.7648197159	2.7619091062
O	1.9529639432	11.7177836590	2.7619091062
O	5.8588918295	11.7177836590	2.7619091062
O	9.7648197159	11.7177836590	2.7619091062
O	13.6707476022	11.7177836590	2.7619091062
O	0.0000000000	13.6707476022	2.7619091062
O	3.9059278863	13.6707476022	2.7619091062
O	7.8118557727	13.6707476022	2.7619091062
O	11.7177836590	13.6707476022	2.7619091062
Ce	13.6707476022	13.6707476022	1.3809540844
Ce	9.7648197159	13.6707476022	1.3809540844
Ce	5.8588918295	13.6707476022	1.3809540844
Ce	1.9529639432	13.6707476022	1.3809540844
Ce	13.6707476022	9.7648197159	1.3809540844
Ce	9.7648197159	9.7648197159	1.3809540844
Ce	5.8588918295	9.7648197159	1.3809540844
Ce	1.9529639432	9.7648197159	1.3809540844
Ce	13.6707476022	5.8588918295	1.3809540844
Ce	9.7648197159	5.8588918295	1.3809540844
Ce	5.8588918295	5.8588918295	1.3809540844
Ce	1.9529639432	5.8588918295	1.3809540844
Ce	13.6707476022	1.9529639432	1.3809540844
Ce	9.7648197159	1.9529639432	1.3809540844
Ce	5.8588918295	1.9529639432	1.3809540844
Ce	1.9529639432	1.9529639432	1.3809540844
O	1.9529639432	0.0000000000	0.0000000000
O	5.8588918295	0.0000000000	0.0000000000
O	9.7648197159	0.0000000000	0.0000000000
O	13.6707476022	0.0000000000	0.0000000000
O	1.9529639432	3.9059278863	0.0000000000
O	5.8588918295	3.9059278863	0.0000000000
O	9.7648197159	3.9059278863	0.0000000000
O	13.6707476022	3.9059278863	0.0000000000
O	1.9529639432	7.8118557727	0.0000000000
O	5.8588918295	7.8118557727	0.0000000000
O	9.7648197159	7.8118557727	0.0000000000
O	13.6707476022	7.8118557727	0.0000000000
O	1.9529639432	11.7177836590	0.0000000000
O	5.8588918295	11.7177836590	0.0000000000
O	9.7648197159	11.7177836590	0.0000000000
O	13.6707476022	11.7177836590	0.0000000000

CH₃+H on CeO₂(100)

C	7.8903311291	5.7833208430	9.5535716058
H	8.1131794857	6.7825145666	9.9659511759
H	6.8828585726	5.4844494434	9.9069134508
H	8.6119733356	5.0587633769	9.9670812702
H	3.8193208255	5.9285569594	9.1819867809
O	0.1442522288	2.0042558226	7.8760530566
O	4.0589991535	2.0680450308	7.8765925277
O	7.9341435473	2.0099863969	7.8816468609
O	11.8318934362	1.9967666121	7.8776138341
O	-0.3496045595	5.8547251263	7.9635837600
O	3.8369985396	5.9146927746	8.1954263592
O	7.9360185958	5.8040791311	8.1203706739
O	11.5486522320	5.8713004312	7.9223119136
O	0.1396830431	9.7210323582	7.8764649445
O	4.0549077878	9.7199713832	7.8790398415
O	7.9356619533	9.6342385627	7.8802912696
O	11.8310689729	9.7548398201	7.8776183025
O	-0.0681446303	13.6875991969	7.8707900688
O	3.8393381279	13.7245165586	7.8676828250
O	7.7436756297	13.6709845671	7.8665822439
O	11.6481288721	13.6883160128	7.8690025131
Ce	13.6509155502	13.6764802232	6.7905365144
Ce	9.7465147723	13.6758161686	6.7892471832
Ce	5.8355698466	13.6798211039	6.7821903745
Ce	1.9307043882	13.6812532515	6.7841980058
Ce	13.6997508198	9.7668765931	6.7847377270
Ce	9.7997365864	9.7609000391	6.7882850438
Ce	5.8899402846	9.7601066670	6.7753829203
Ce	1.9794698198	9.7636035037	6.7747890630
Ce	13.6059994419	5.8618911915	6.7749769225
Ce	9.8449202976	5.8598649368	6.7342920121
Ce	5.8443703865	5.8575985456	6.7783672679
Ce	1.7841742692	5.8605930955	6.8210216722
Ce	13.6990838279	1.9603216020	6.7846390788
Ce	9.7988896249	1.9578880527	6.7880369705
Ce	5.8918346753	1.9659492473	6.7765005781
Ce	1.9800405852	1.9665940223	6.7753983253
O	1.9491601162	0.0036063901	5.6168234643
O	5.8551542315	0.0056610644	5.6147504165
O	9.7622979395	-0.0005255973	5.6260651084
O	13.6698185226	-0.0042105903	5.6262067842
O	-0.0374126334	1.9385576625	5.3040133236
O	3.8838980469	1.9505052241	5.3050880631
O	7.8193687625	1.9501871097	5.3048922511
O	11.7101104168	1.9276999954	5.3020743585
O	1.9143891869	3.8808519856	5.5806726018
O	5.8752412312	3.8897304721	5.5604793296
O	9.8015023157	3.8847116360	5.5870068451
O	13.6406720512	3.8777220093	5.5953731082

O	-0.0861733310	5.8635167450	5.2980174899
O	3.8754557274	5.8637586000	5.3818247660
O	7.8888044269	5.8637090260	5.3914548156
O	11.7399694857	5.8609250056	5.3041139246
O	1.9112209638	7.8457504775	5.5836491376
O	5.8789638149	7.8357715817	5.5665995905
O	9.7990441435	7.8382853587	5.5855209988
O	13.6428180461	7.8470580884	5.5978636528
O	-0.0339778542	9.7904744439	5.3038170429
O	3.8865229554	9.7697789944	5.3054596887
O	7.8170136442	9.7840864551	5.3051076708
O	11.7097742258	9.7912976417	5.3006149476
O	1.9535538633	11.7262163386	5.6252777514
O	5.8545112845	11.7240586416	5.6218904839
O	9.7610249976	11.7259323620	5.6329305734
O	13.6700001795	11.7304640821	5.6276244173
O	0.0087864941	13.6740278630	5.2976127108
O	3.9085101734	13.6722007949	5.2998323559
O	7.8132893888	13.6763496402	5.2975120785
O	11.7243334783	13.6722037634	5.2992044076
Ce	11.7181568314	11.7251183979	4.0984797726
Ce	7.8120694738	11.7229003308	4.0958448805
Ce	3.9045333920	11.7173442265	4.0929708988
Ce	0.0000760719	11.7222913967	4.0966631256
Ce	11.7269362792	7.8334094640	4.0845523118
Ce	7.8130639543	7.8161058909	4.1024084330
Ce	3.8917465715	7.7971187693	4.1152179391
Ce	-0.0077971382	7.8152645697	4.0958350376
Ce	11.7264291804	3.8859006630	4.0849202346
Ce	7.8135457583	3.9071134917	4.1009714890
Ce	3.8923493811	3.9228904719	4.1137762143
Ce	-0.0087513408	3.9074102797	4.0951982620
Ce	11.7180399817	-0.0050233514	4.0974799488
Ce	7.8124826273	0.0005203321	4.0944994134
Ce	3.9040924596	0.0035886884	4.0918943001
Ce	-0.0006155586	0.0012282268	4.0967708354
O	1.9529639432	0.0000000000	2.7619091062
O	5.8588918295	0.0000000000	2.7619091062
O	9.7648197159	0.0000000000	2.7619091062
O	13.6707476022	0.0000000000	2.7619091062
O	0.0000000000	1.9529639432	2.7619091062
O	3.9059278863	1.9529639432	2.7619091062
O	7.8118557727	1.9529639432	2.7619091062
O	11.7177836590	1.9529639432	2.7619091062
O	1.9529639432	3.9059278863	2.7619091062
O	5.8588918295	3.9059278863	2.7619091062
O	9.7648197159	3.9059278863	2.7619091062
O	13.6707476022	3.9059278863	2.7619081687
O	0.0000000000	5.8588918295	2.7619091062
O	3.9059278863	5.8588918295	2.7619091062
O	7.8118557727	5.8588918295	2.7619091062

O	11.7177836590	5.8588918295	2.7619091062
O	1.9529639432	7.8118557727	2.7619091062
O	5.8588918295	7.8118557727	2.7619091062
O	9.7648197159	7.8118557727	2.7619091062
O	13.6707476022	7.8118557727	2.7619091062
O	0.0000000000	9.7648197159	2.7619091062
O	3.9059278863	9.7648197159	2.7619091062
O	7.8118557727	9.7648197159	2.7619091062
O	11.7177836590	9.7648197159	2.7619091062
O	1.9529639432	11.7177836590	2.7619091062
O	5.8588918295	11.7177836590	2.7619091062
O	9.7648197159	11.7177836590	2.7619091062
O	13.6707476022	11.7177836590	2.7619091062
O	0.0000000000	13.6707476022	2.7619091062
O	3.9059278863	13.6707476022	2.7619091062
O	7.8118557727	13.6707476022	2.7619091062
O	11.7177836590	13.6707476022	2.7619091062
Ce	13.6707476022	13.6707476022	1.3809540844
Ce	9.7648197159	13.6707476022	1.3809540844
Ce	5.8588918295	13.6707476022	1.3809540844
Ce	1.9529639432	13.6707476022	1.3809540844
Ce	13.6707476022	9.7648197159	1.3809540844
Ce	9.7648197159	9.7648197159	1.3809540844
Ce	5.8588918295	9.7648197159	1.3809540844
Ce	1.9529639432	9.7648197159	1.3809540844
Ce	13.6707476022	5.8588918295	1.3809540844
Ce	9.7648197159	5.8588918295	1.3809540844
Ce	5.8588918295	5.8588918295	1.3809540844
Ce	1.9529639432	5.8588918295	1.3809540844
Ce	13.6707476022	1.9529639432	1.3809540844
Ce	9.7648197159	1.9529639432	1.3809540844
Ce	5.8588918295	1.9529639432	1.3809540844
Ce	1.9529639432	1.9529639432	1.3809540844
O	1.9529639432	0.0000000000	0.0000000000
O	5.8588918295	0.0000000000	0.0000000000
O	9.7648197159	0.0000000000	0.0000000000
O	13.6707476022	0.0000000000	0.0000000000
O	1.9529639432	3.9059278863	0.0000000000
O	5.8588918295	3.9059278863	0.0000000000
O	9.7648197159	3.9059278863	0.0000000000
O	13.6707476022	3.9059278863	0.0000000000
O	1.9529639432	7.8118557727	0.0000000000
O	5.8588918295	7.8118557727	0.0000000000
O	9.7648197159	7.8118557727	0.0000000000
O	13.6707476022	7.8118557727	0.0000000000
O	1.9529639432	11.7177836590	0.0000000000
O	5.8588918295	11.7177836590	0.0000000000
O	9.7648197159	11.7177836590	0.0000000000
O	13.6707476022	11.7177836590	0.0000000000

CH₄ on Ag:CeO_{2-x}(100)

C	5.3273233293	9.6554789176	9.1100865618
H	6.0505140283	10.2733537917	9.6593535325
H	4.6505527432	9.1528379808	9.8143749304
H	5.8718613144	8.8864715077	8.5381722301
H	4.7460396189	10.3078429342	8.4360224826
O	0.0149290575	1.9877279007	7.8788687447
O	3.9278256427	2.0028419588	7.8738093450
O	7.8102613528	2.1953707851	7.8600033808
O	11.7273678911	2.0227980130	7.8779540744
O	-0.0600507153	5.9328906908	7.8895985900
O	3.6916806551	6.0947026246	7.9110325260
O	7.9829394758	6.1567283135	7.8964378920
O	11.7553812213	5.8983118572	7.8885879180
O	0.0981651109	9.7658367282	7.9248877460
O	9.4239877435	11.5762863585	7.9373453267
O	11.9428001340	9.6667659160	7.9301471331
O	-0.0001140323	13.6541587835	7.8859339750
O	3.8058532856	13.5621073012	7.8874918349
O	7.6057023345	14.1050808838	7.8575784526
O	11.7656273456	13.7949100271	7.8762635783
Ce	13.6465491455	13.6903109376	6.8114836923
Ce	9.7225838668	13.5383763155	6.9079282567
Ce	5.8217911786	13.6811869409	6.8304871290
Ce	1.9072736576	13.6848302125	6.8025365813
Ce	13.6925676656	9.7581851758	6.7699777397
Ce	9.9974640830	9.9136930220	6.7982109486
Ag	5.8662793536	9.7779156210	5.9554027910
Ce	1.7571833693	9.7588857935	6.6769093540
Ce	13.6539850815	5.8612675195	6.8074239233
Ce	9.7992953673	5.8916500650	6.7999091949
Ce	5.8679199389	5.9018052074	6.8447568645
Ce	1.8999275511	5.8675736346	6.8143492933
Ce	13.6647052616	1.9637038573	6.8154860881
Ce	9.7691019340	1.9393333249	6.8011013962
Ce	5.8800031721	1.9578586123	6.8020101816
Ce	1.9559002931	1.9668223086	6.8106009659
O	1.9431245495	0.0249567333	5.6489661726
O	5.8327577428	-0.0082871598	5.6150566478
O	9.7611131623	-0.0317142129	5.6622482350
O	13.6847327864	0.0269689147	5.6441322164
O	0.0000966725	1.9617161869	5.2981209242
O	3.9053304402	1.9586837504	5.2958342928
O	7.8136033554	1.9211060761	5.2962193528
O	11.7062678935	1.9408848184	5.3001016933
O	1.9520682523	3.8999414919	5.6379740073
O	5.8641811187	3.9100400242	5.6393885054
O	9.7704940394	3.8907472377	5.6317695630
O	13.6625726336	3.8924691366	5.6375632975
O	-0.0220956059	5.8418189295	5.2872070591

O	3.8820672207	5.8686587025	5.2968970801
O	7.8523067444	5.8573344792	5.2943625191
O	11.7357012192	5.8558990699	5.2881259567
O	1.8874943597	7.8189957301	5.5756485084
O	5.8699507345	7.7755853675	5.5644468048
O	9.8288931059	7.8485539670	5.5877623896
O	13.6890555231	7.8111710040	5.6018279355
O	-0.0090623351	9.7627865520	5.3005204230
O	3.8187899187	9.7548445498	5.5790804014
O	7.8927084239	9.7782340655	5.5588186457
O	11.7918235276	9.7928980151	5.3240439190
O	1.8952959534	11.7112500822	5.6006745941
O	5.8182670573	11.7823471146	5.5655672550
O	9.8551019049	11.7321104727	5.3815924640
O	13.7145189086	11.7226858590	5.6407630818
O	-0.0078843216	13.6911743635	5.2854152118
O	3.8432973108	13.6779440216	5.2851915452
O	7.8322884134	13.6150937044	5.3207868057
O	11.7778040397	13.6725415375	5.3005841184
Ce	11.7397664808	11.7543883853	4.0761237702
Ce	7.8668073845	11.7517703110	4.0833815509
Ce	3.8794234322	11.7721251280	4.0781870729
Ce	-0.0272820609	11.7611262995	4.0788112107
Ce	11.7217116824	7.8070662961	4.1043226710
Ce	7.8700442028	7.7768138295	4.1000391512
Ce	3.8780842469	7.7590854290	4.0792321386
Ce	-0.0299135654	7.7715481248	4.0694062356
Ce	11.7133845136	3.8943481530	4.1064917236
Ce	7.8169888496	3.8933037565	4.1139226473
Ce	3.9107849943	3.8998098934	4.1174037568
Ce	-0.0047085380	3.8938838143	4.1076276206
Ce	11.7014891358	-0.0107831295	4.1310771794
Ce	7.8258649194	-0.0213384221	4.1330856291
Ce	3.9070895214	0.0167727772	4.1063655459
Ce	-0.0101227784	0.0186566709	4.1076931145
O	1.9529639432	0.0000000000	2.7619091062
O	5.8588918295	0.0000000000	2.7619091062
O	9.7648197159	0.0000000000	2.7619091062
O	13.6707476022	0.0000000000	2.7619091062
O	0.0000000000	1.9529639432	2.7619091062
O	3.9059278863	1.9529639432	2.7619091062
O	7.8118557727	1.9529639432	2.7619091062
O	11.7177836590	1.9529639432	2.7619091062
O	1.9529639432	3.9059278863	2.7619091062
O	5.8588918295	3.9059278863	2.7619091062
O	9.7648197159	3.9059278863	2.7619091062
O	13.6707476022	3.9059278863	2.7619081687
O	0.0000000000	5.8588918295	2.7619091062
O	3.9059278863	5.8588918295	2.7619091062
O	7.8118557727	5.8588918295	2.7619091062
O	11.7177836590	5.8588918295	2.7619091062

O	1.9529639432	7.8118557727	2.7619091062
O	5.8588918295	7.8118557727	2.7619091062
O	9.7648197159	7.8118557727	2.7619091062
O	13.6707476022	7.8118557727	2.7619091062
O	0.0000000000	9.7648197159	2.7619091062
O	3.9059278863	9.7648197159	2.7619091062
O	7.8118557727	9.7648197159	2.7619091062
O	11.7177836590	9.7648197159	2.7619091062
O	1.9529639432	11.7177836590	2.7619091062
O	5.8588918295	11.7177836590	2.7619091062
O	9.7648197159	11.7177836590	2.7619091062
O	13.6707476022	11.7177836590	2.7619091062
O	0.0000000000	13.6707476022	2.7619091062
O	3.9059278863	13.6707476022	2.7619091062
O	7.8118557727	13.6707476022	2.7619091062
O	11.7177836590	13.6707476022	2.7619091062
Ce	13.6707476022	13.6707476022	1.3809540844
Ce	9.7648197159	13.6707476022	1.3809540844
Ce	5.8588918295	13.6707476022	1.3809540844
Ce	1.9529639432	13.6707476022	1.3809540844
Ce	13.6707476022	9.7648197159	1.3809540844
Ce	9.7648197159	9.7648197159	1.3809540844
Ce	5.8588918295	9.7648197159	1.3809540844
Ce	1.9529639432	9.7648197159	1.3809540844
Ce	13.6707476022	5.8588918295	1.3809540844
Ce	9.7648197159	5.8588918295	1.3809540844
Ce	5.8588918295	5.8588918295	1.3809540844
Ce	1.9529639432	5.8588918295	1.3809540844
Ce	13.6707476022	1.9529639432	1.3809540844
Ce	9.7648197159	1.9529639432	1.3809540844
Ce	5.8588918295	1.9529639432	1.3809540844
Ce	1.9529639432	1.9529639432	1.3809540844
O	1.9529639432	0.0000000000	0.0000000000
O	5.8588918295	0.0000000000	0.0000000000
O	9.7648197159	0.0000000000	0.0000000000
O	13.6707476022	0.0000000000	0.0000000000
O	1.9529639432	3.9059278863	0.0000000000
O	5.8588918295	3.9059278863	0.0000000000
O	9.7648197159	3.9059278863	0.0000000000
O	13.6707476022	3.9059278863	0.0000000000
O	1.9529639432	7.8118557727	0.0000000000
O	5.8588918295	7.8118557727	0.0000000000
O	9.7648197159	7.8118557727	0.0000000000
O	13.6707476022	7.8118557727	0.0000000000
O	1.9529639432	11.7177836590	0.0000000000
O	5.8588918295	11.7177836590	0.0000000000
O	9.7648197159	11.7177836590	0.0000000000
O	13.6707476022	11.7177836590	0.0000000000

CH₃+H on Ag:CeO_{2-x}(100)

C	8.0018181961	5.7932993704	9.4967738729
H	8.2143438584	6.6598090921	10.1475157923
H	7.0059115093	5.3895394373	9.7742456657
H	8.7366039028	4.9968848137	9.7205061958
H	3.5916738491	6.2340482227	9.1064041373
O	0.0172912758	2.0084295860	7.8816657978
O	3.9324587500	2.1518889701	7.8656897831
O	7.7972235507	2.3089929946	7.8455091866
O	11.7069188925	2.0241210353	7.8799231830
O	-0.0214837584	5.8771738601	7.8932431865
O	3.6818507577	6.2480800469	8.1221390736
O	8.0344485214	6.1631396277	8.1127850901
O	11.7574873534	5.8321442186	7.8930657893
O	0.0682075366	9.7272164746	7.9124339506
O	9.3616465046	11.5644757474	7.9256992702
O	11.9345043505	9.6303249910	7.9158275114
O	-0.0072530092	13.6642177461	7.8956904124
O	3.8001002614	13.5519786181	7.8890466296
O	7.6135423202	14.1350606962	7.8441289351
O	11.7615886963	13.7834945727	7.8812053604
Ce	13.6423734185	13.6869679288	6.8207451046
Ce	9.6923149983	13.5368776056	6.9316570226
Ce	5.8189428609	13.6604177207	6.7888384833
Ce	1.9081375312	13.6897868027	6.8102402990
Ce	13.6865697355	9.7606052516	6.7707831892
Ce	9.9788891787	9.9214131993	6.7573815582
Ag	5.8956794194	9.7757016063	6.4335788591
Ce	1.7547015000	9.7661332979	6.6537829707
Ce	13.6570149629	5.8530884313	6.7569554151
Ce	9.9189421308	5.8600207233	6.7181417937
Ce	5.8762928943	5.9092514022	6.7497161889
Ce	1.7839114454	5.8506652527	6.7206041018
Ce	13.6601325469	1.9563535380	6.8159040576
Ce	9.7654019796	1.9293963507	6.7904751168
Ce	5.8776121285	1.9798222665	6.7759307697
Ce	1.9490975160	1.9678803266	6.8031237511
O	1.9296558833	0.0395881521	5.6552157165
O	5.8269806800	0.0112649755	5.6131006277
O	9.7655636357	-0.0240419864	5.6624697044
O	13.6881885700	0.0371189795	5.6565304731
O	-0.0185937364	1.9622019657	5.2974592400
O	3.8814038735	1.9717054475	5.2948294921
O	7.8283884700	1.9313595763	5.2946286447
O	11.7210009851	1.9408369530	5.3009389697
O	1.8961547444	3.8972643238	5.6204908409
O	5.8642641914	3.9153570041	5.5641622999
O	9.8139185843	3.8856439063	5.6118279648
O	13.6635630322	3.8892818340	5.6364296014

O	-0.0601661619	5.8287976153	5.2875501822
O	3.7825329583	5.8459153845	5.4140454270
O	7.9299423816	5.8562286900	5.4009213189
O	11.7760107975	5.8370301662	5.2873383636
O	1.8201370596	7.7746287513	5.5921790487
O	5.8508133109	7.7297005577	5.4424110830
O	9.9043493351	7.7879716510	5.6251164204
O	13.6884907082	7.7958557817	5.6011692809
O	-0.0206183422	9.7626322363	5.2835575919
O	3.6806332084	9.7274459405	5.4779786706
O	8.0467589043	9.7399666955	5.4482970979
O	11.7913427064	9.7911919276	5.3050592014
O	1.8617869625	11.7389780906	5.6181840315
O	5.8026305297	11.8104117739	5.5100769743
O	9.8813166624	11.7847128705	5.3913556367
O	13.7133736235	11.7247097290	5.6448125765
O	-0.0205296107	13.7047474610	5.2877176946
O	3.8205848992	13.6986270165	5.2899195087
O	7.8321141775	13.6247001113	5.3216630885
O	11.8089327377	13.6935931652	5.2945571241
Ce	11.7341406373	11.7659716346	4.0749804612
Ce	7.8331217960	11.7118639435	4.1210961111
Ce	3.9148407537	11.7340834416	4.1179591008
Ce	-0.0198565357	11.7695610414	4.0793338533
Ce	11.7213592759	7.8288835213	4.0790524218
Ce	7.8393786131	7.8324450707	4.1304468875
Ce	3.9111974183	7.8102471827	4.1104567962
Ce	-0.0277262248	7.7968705761	4.0421344930
Ce	11.7224667491	3.8675520644	4.0805633791
Ce	7.8216494995	3.8999710145	4.0981547662
Ce	3.9033169186	3.9044013147	4.1021344726
Ce	-0.0153644201	3.8685838629	4.0809575843
Ce	11.7014782861	-0.0218632461	4.1349511293
Ce	7.8246838404	-0.0369766322	4.1263036093
Ce	3.9045028132	0.0033223698	4.0989368429
Ce	-0.0120412239	0.0082826886	4.1116271661
O	1.9529639432	0.0000000000	2.7619091062
O	5.8588918295	0.0000000000	2.7619091062
O	9.7648197159	0.0000000000	2.7619091062
O	13.6707476022	0.0000000000	2.7619091062
O	0.0000000000	1.9529639432	2.7619091062
O	3.9059278863	1.9529639432	2.7619091062
O	7.8118557727	1.9529639432	2.7619091062
O	11.7177836590	1.9529639432	2.7619091062
O	1.9529639432	3.9059278863	2.7619091062
O	5.8588918295	3.9059278863	2.7619091062
O	9.7648197159	3.9059278863	2.7619091062
O	13.6707476022	3.9059278863	2.7619081687
O	0.0000000000	5.8588918295	2.7619091062
O	3.9059278863	5.8588918295	2.7619091062
O	7.8118557727	5.8588918295	2.7619091062

O	11.7177836590	5.8588918295	2.7619091062
O	1.9529639432	7.8118557727	2.7619091062
O	5.8588918295	7.8118557727	2.7619091062
O	9.7648197159	7.8118557727	2.7619091062
O	13.6707476022	7.8118557727	2.7619091062
O	0.0000000000	9.7648197159	2.7619091062
O	3.9059278863	9.7648197159	2.7619091062
O	7.8118557727	9.7648197159	2.7619091062
O	11.7177836590	9.7648197159	2.7619091062
O	1.9529639432	11.7177836590	2.7619091062
O	5.8588918295	11.7177836590	2.7619091062
O	9.7648197159	11.7177836590	2.7619091062
O	13.6707476022	11.7177836590	2.7619091062
O	0.0000000000	13.6707476022	2.7619091062
O	3.9059278863	13.6707476022	2.7619091062
O	7.8118557727	13.6707476022	2.7619091062
O	11.7177836590	13.6707476022	2.7619091062
Ce	13.6707476022	13.6707476022	1.3809540844
Ce	9.7648197159	13.6707476022	1.3809540844
Ce	5.8588918295	13.6707476022	1.3809540844
Ce	1.9529639432	13.6707476022	1.3809540844
Ce	13.6707476022	9.7648197159	1.3809540844
Ce	9.7648197159	9.7648197159	1.3809540844
Ce	5.8588918295	9.7648197159	1.3809540844
Ce	1.9529639432	9.7648197159	1.3809540844
Ce	13.6707476022	5.8588918295	1.3809540844
Ce	9.7648197159	5.8588918295	1.3809540844
Ce	5.8588918295	5.8588918295	1.3809540844
Ce	1.9529639432	5.8588918295	1.3809540844
Ce	13.6707476022	1.9529639432	1.3809540844
Ce	9.7648197159	1.9529639432	1.3809540844
Ce	5.8588918295	1.9529639432	1.3809540844
Ce	1.9529639432	1.9529639432	1.3809540844
O	1.9529639432	0.0000000000	0.0000000000
O	5.8588918295	0.0000000000	0.0000000000
O	9.7648197159	0.0000000000	0.0000000000
O	13.6707476022	0.0000000000	0.0000000000
O	1.9529639432	3.9059278863	0.0000000000
O	5.8588918295	3.9059278863	0.0000000000
O	9.7648197159	3.9059278863	0.0000000000
O	13.6707476022	3.9059278863	0.0000000000
O	1.9529639432	7.8118557727	0.0000000000
O	5.8588918295	7.8118557727	0.0000000000
O	9.7648197159	7.8118557727	0.0000000000
O	13.6707476022	7.8118557727	0.0000000000
O	1.9529639432	11.7177836590	0.0000000000
O	5.8588918295	11.7177836590	0.0000000000
O	9.7648197159	11.7177836590	0.0000000000
O	13.6707476022	11.7177836590	0.0000000000

CH₃OH on Ag:CeO_{2-x}(100)

C	7.6923256146	5.3740905255	9.4302112991
H	7.8935054985	5.0356481113	10.4552604834
H	6.7894898823	6.0111437184	9.4662699091
H	7.5642941140	4.4740641814	8.7939804702
H	9.5594504505	6.1404599729	9.5604155407
O	0.0192955244	2.0271089384	7.8798047239
O	3.9729253168	2.1735176769	7.8649832747
O	7.8239663435	2.4529809160	7.8236621497
O	11.6947161856	2.0670201102	7.8789679796
O	-0.1333243350	5.9186324675	7.9233279725
O	3.5399612206	6.2474014415	7.9552253787
O	8.7968804706	6.1829960994	8.9249724696
O	11.7202679238	5.8517379408	7.9113804210
O	0.0664213629	9.7509465679	7.9092355959
O	9.3653654855	11.5773472408	7.9236050004
O	11.9311040387	9.6281638817	7.9149772362
O	-0.0073290880	13.6865734541	7.8980798391
O	3.8115857934	13.5825917075	7.8889763366
O	7.6245621054	14.1888268061	7.8323273107
O	11.7618026385	13.8124037116	7.8800362859
Ce	13.6472505282	13.6919042401	6.8209020741
Ce	9.6980314102	13.5494393074	6.9247114611
Ce	5.8247864557	13.6711188579	6.7887340880
Ce	1.9093245780	13.6935341407	6.8119484681
Ce	13.6978839812	9.7615559252	6.7699568491
Ce	9.9937958333	9.9347406084	6.7548270242
Ag	5.8794514721	9.7786360268	6.4299122385
Ce	1.7651634453	9.7564585668	6.6568737500
Ce	13.6936727961	5.8603083201	6.7704968606
Ce	9.9888945766	5.8441032320	6.6509344077
Ce	5.5748372196	5.9047071918	6.7455908460
Ce	1.8245494962	5.8735809258	6.8035142705
Ce	13.6699120493	1.9634723345	6.8112461080
Ce	9.7779781961	1.9388004944	6.7836848168
Ce	5.8711754027	1.9878333658	6.7685120468
Ce	1.9542774748	1.9802654578	6.7976885870
O	1.9292547075	0.0405150869	5.6591233173
O	5.8309163567	0.0120831108	5.6069850198
O	9.7647390053	-0.0160487465	5.6568990267
O	13.6924269966	0.0383222445	5.6566949685
O	-0.0116236236	1.9598572870	5.3001208619
O	3.8787843917	1.9551646295	5.2976755530
O	7.8200014639	1.9342884413	5.2954050092
O	11.7330890550	1.9344168241	5.3016310367
O	1.9089311487	3.8893925855	5.6282930770
O	5.8424720707	3.9135491125	5.5612999304
O	9.8266503709	3.8764287252	5.5697935924
O	13.6691150162	3.8824983287	5.6308236111

O	-0.0534583040	5.8297919840	5.2967656040
O	3.7868677272	5.8280592984	5.3133666976
O	7.9235495136	5.8643913627	5.5720832893
O	11.7901152549	5.8344585819	5.2804718101
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Ce	-0.0159103378	11.7669365927	4.0820574387
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Ce	-0.0209147545	7.7882371630	4.0577937131
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Ce	11.7044542342	-0.0229085585	4.1342019767
Ce	7.8246706891	-0.0355924253	4.1231563606
Ce	3.9034910486	-0.0007099984	4.1001097686
Ce	-0.0095262600	0.0103683857	4.1107803084
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O	5.8588918295	0.0000000000	2.7619091062
O	9.7648197159	0.0000000000	2.7619091062
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