Ab Initio study of adsorption of fission gas atoms Xe and Kr on MoS_2 monolayer functionalized with 3d transition metals

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I. RESULTS AND DISCUSSION

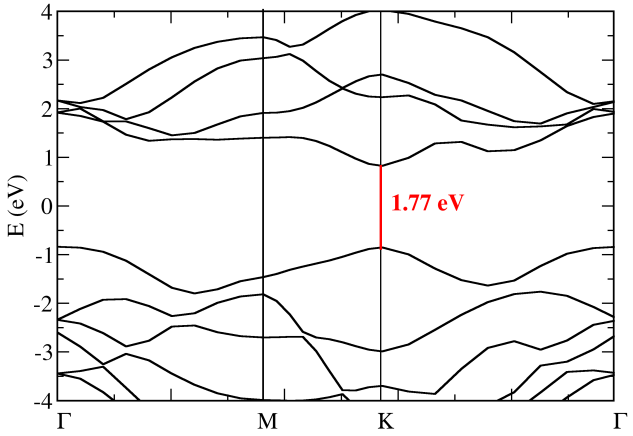


FIG. S1. The band structure of the electron levels for a single MoS_2 monolayer. Red line depicts the direct band gap of 1.77 eV.

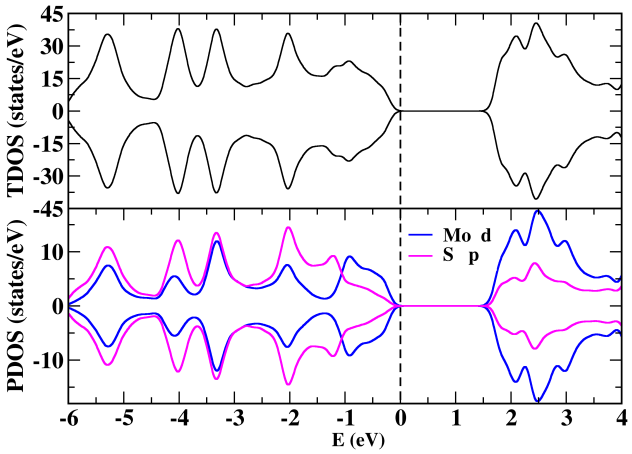
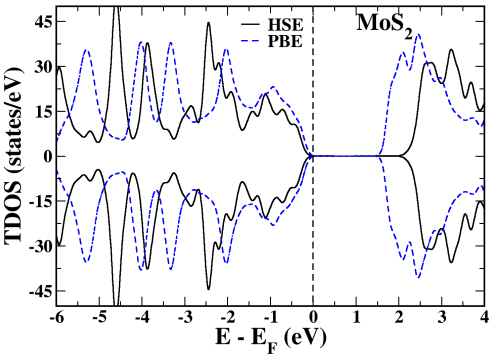
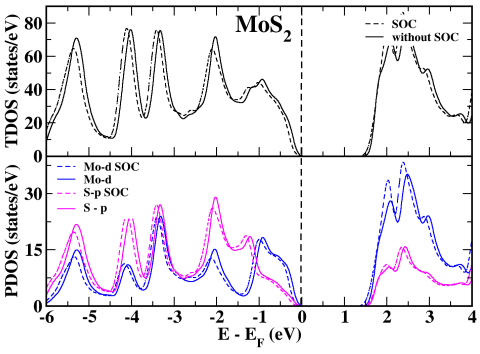


FIG. S2. Upper panel depicts the total density of states (TDOS), lower panel shows partial desity of states (PDOS) of d orbital of Mo and p orbital of S atoms. Fermi level is set to zero and indicated by a vertical black dashed line. DOS is broadened by Gaussian smearing with 0.2 eV.



(a) Plot of total density of states (TDOS) with HSE06 and PBE potential for pristine MoS_2 monolayer.



(b) Upper panel displays total density of states (TDOS) with/without spin orbit coupling (SOC) correactions while lower panels represents partial DOS (PDOS) with/without SOC for pristine MoS_2 monolayer.

FIG. S3. (a) TDOS with HSE06 and PBE potential and (b) TDOS and PDOS with/without SOC correactions for MoS_2 surface. Fermi level is set to zero and indicated by a vertical black dashed line. DOS is broadened by Gaussian smearing with 0.2 eV.

A. Properties of TM functionalized MoS_2 monolayer

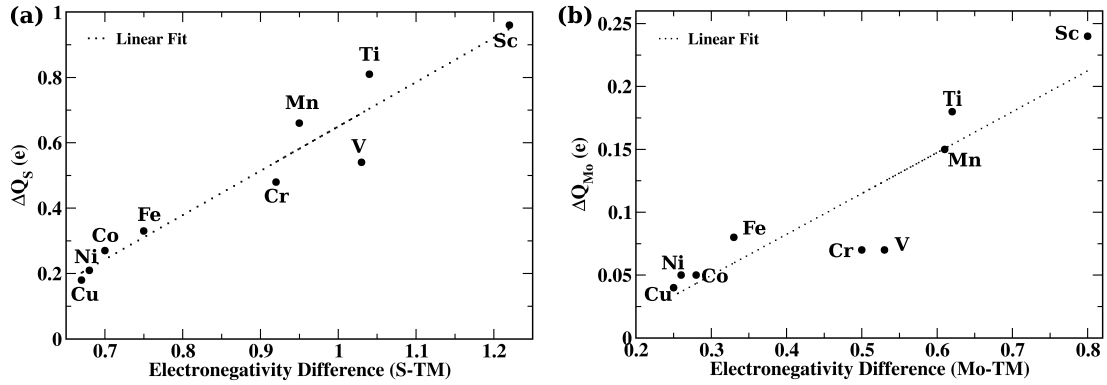
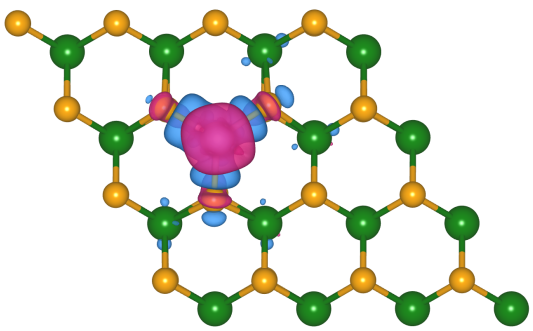
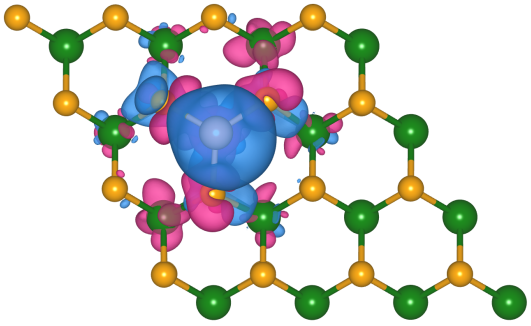


FIG. S4. Plot of the electronic charge transfer versus electronegativity difference (on Pauling scale). Plot (a) represents the charge transfer of S atoms versus the electronegativity difference between the S and the TM atoms. Plot (b) shows the charge transfer in Mo atoms versus the electronegativity difference between the Mo and the TM atoms. The dotted line traces a linear regression fit. Positive sign of ΔQ denotes that charge is gained by the S and Mo atoms.

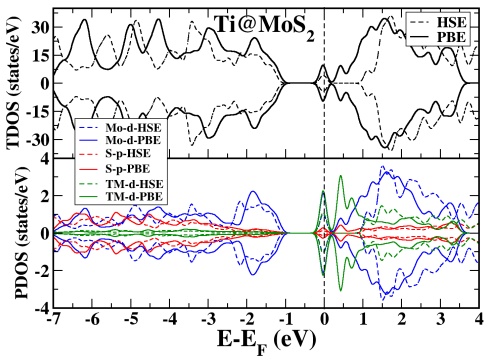


(a) Top views of charge density difference $\Delta\rho(r) = \rho^{MoS_2+TM}(r) - \left(\rho^{MoS_2}(r) + \rho^{TM}(r)\right)$ for functionalized Mn–MoS_2 monolayer for second most configuration. The blue and magenta regions represent positive $\Delta\rho(r)$ and negative $\Delta\rho(r)$, respectively. The isosurface value is 0.004 e/Å^3.

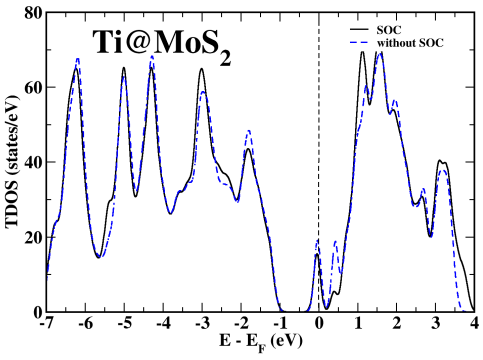


(b) Top views of spin density $(\rho(\uparrow) - \rho(\downarrow))$ for MoS_2 monolayer, functionalized with Mn metal atom for the second most configuration. The blue and magenta regions represent positive spin density and negative spin density, respectively. The isosurface value is 0.001 e/Å^3.

FIG. S5. (a) Charge density difference and (b) spin density plots for Mn functionalized MoS_2 surface for the second most stable configuration.



(a) Upper panel depicts the total density of states (TDOS), lower panel shows partial desity of states (PDOS) of d orbital of Mo, p orbital of S, and d orbital of Ti atoms with HSE06 and PBE potential for Ti functionalized MoS_2 surface.



(b) Plot displays total density of states (TDOS) with/without spin orbit coupling (SOC) correactions for Ti functionalized MoS_2 surface.

FIG. S6. (a) TDOS/PDOS with HSE06 and PBE potential and (b) TDOS with/without SOC correactions for Ti functionalized MoS_2 surface. Fermi level is set to zero and indicated by a vertical black dashed line. DOS is broadened by Gaussian smearing with 0.2 eV.

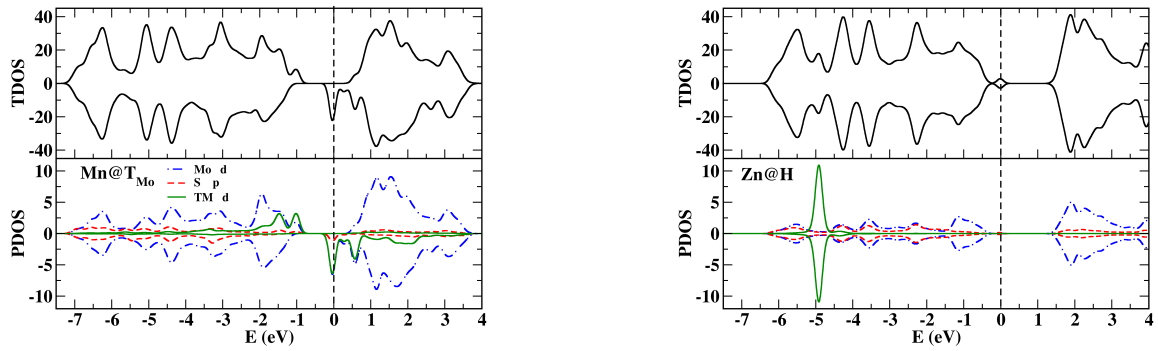


FIG. S7. Spin-polarized density of states for functionalized MoS_2 with Mn and Zn transition metals for the second most configuration. In each of the figures, upper panel exhibits the total density of states (TDOS) and lower panel shows the partial density of states (PDOS) of the d electronic orbitals of the TM atom, p electronic orbitals of sulfur atoms (neighboring to TM adatom: H site and T_{Mo} have PDOS of nearest neighboring 3 S atoms) and d electronic orbitals of molybdenum atoms (neighboring to TM adatom: H site has PDOS for neighboring 3 Mo atoms and T_{Mo} site has PDOS for neighboring 1 Mo atom and next neighboring 6 Mo atoms). Fermi level is set to zero and indicated by a vertical black dashed line.

TABLE S1. The second most favorable site for *3d* transition metal (TM) atom adsorption on surface is shown in the 2nd column, d_{TM-S} shows the average bond distances between the TM and its nearest neighbor S atoms. Columns of magentic moment display total magnetic moment (M_{Tot}) of TM-MoS_2 system, magnetic moment of the adatom (M_{TM}), sum of magnetic moment of the nearest neighbor S atoms (M_{NN-S}), Mo atoms (M_{NN-Mo}) and of next nearest neighbor Mo (M_{NNN-Mo}). Last 3 coloumns represent Bader charge (ΔQ) on TM adatom, the neighboring S atoms and Mo atoms. For **H** site, there are 3 Mo and 3 S nearest neighbor atoms and $\mathbf{T_{Mo}}$ site has 3 S and 1 Mo atoms as nearest neighbors and 6 Mo atoms as next nearest neighbors. Positive sign indicates that charge is donated, while negative sign indicates that charge is accepted.

			Magnetic Moment					Charge Transfer		
TM	Site	d_{TM-S}	M_{Tot}	M_{TM}	M_{NN-S}	M_{NN-Mo}	M_{NNN-Mo}	ΔQ_{TM}	ΔQ_{NN-S}	ΔQ_{NN-Mo}
		(Å)	(μ_B)	(μ_B)	(μ_B)	(μ_B)	(μ_B)	(e)	(e)	(e)
Mn	T_{Mo}	2.19	2.99	2.85	-0.10	-0.08	-0.08	0.85	-0.47	-0.11
Zn	H	3.10	0.00	0.00	0.00	0.00	0.00	0.03	-0.08	-0.06

B. Adsorption of Xe and Kr atoms on pristine and *3d* TM functionalized MoS_2 monolayer

TABLE S2. Adsorption energy of Xe and Kr gas atoms on the second most stable configured TM functionalized MoS_2 monolayer with Mn, and Zn TM atoms.

Site	Xe	Kr
	E_{ads}(meV)	E_{ads}(meV)
Mn	-456.84	-315.25
Zn	-68.44	-49.19

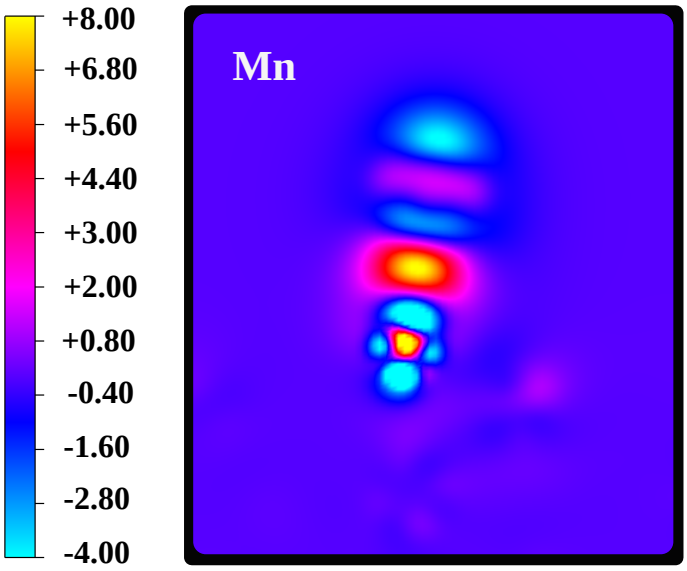


FIG. S8. Charge density difference (CDD), $\Delta\rho(r) = \rho^{MoS_2+TM+Xe}(r) - \rho^{TM+MoS_2}(r) - \rho^{Xe}(r)$, plotted for Xe adsorption on the secondmost stable configured functionalized MoS_2 surface with Mn metal atoms. Plots are in units of 0.001 e/Å^3. Magenta, red and yellow (cyan and blue) colors indicate accumulation (depletion) of electron charge density.

The simulation of surfaces of periodic crystals has various challenges for the DFT based first-principles calculations. To calculate the surface's properties, one may use both sides of the surfaces of a slab if they are equivalent. A subtle problem may arise while simulating an adatom's adsorption on one side of the slab with periodic boundary conditions, which is nowadays a common practice. However, due to such geometry, the slab acquires a dipole moment, and because of the periodic boundary conditions, an array of dipole moments is created. This array causes an electric field to generate, distorting the slab's electron density and changing the energy. Moreover, because of the existence of this field in the vacuum, the zero-potential in the vacuum becomes ill-defined; thus, leading to the wrong estimation of the work function. To handle this, a dipole correction scheme was developed by Makov, Neugebauer and Scheffler.[1,2] In this method, an external field is applied in the vacuum region, which cancels the artificial field induced by the dipole moment of the slab. The benefit of this method is that the one-sided adsorbate slabs can be simulated accurately.

TABLE S3. Adsorption energy of Xe and Kr on pristine and functionalized MoS_2 without and with dipole correction (developed by Makov, Neugebauer and Scheffler method which is implemented in VASP software). E_{ads} represents the adsorption energy without dipole correction while E_{ads}(dip-corr) display adsorption energy after dipole correction is included.

	Xe		**Kr**	
System	E_{ads} [meV]	E_{ads}(dip-corr) [meV]	E_{ads} [meV]	E_{ads}(dip-corr) [meV]
MoS_2	-187	-186	-138	-138
Sc-MoS_2	-406	-362	-312	-280
Ti-MoS_2	-518	-484	-395	-370
V-MoS_2	-490	-456	-363	-337
Cr-MoS_2	-355	-312	-218	-183
Mn-MoS_2	-392	-371	-260	-246
Fe-MoS_2	-417	-389	-279	-260
Co-MoS_2	-466	-447	-308	-295
Ni-MoS_2	-461	-445	-293	-281
Cu-MoS_2	-254	-234	-159	-131

II. STRUCTURE FILES

Pristine MoS_2

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0.0000006632577292 0.0000011370140710 19.4620012899153885

Mo S

16 32

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Xe-MoS$_2$@T$_{Mo}$

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Mo S Xe

16 32 1

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Kr-MoS_2@T_{Mo}

1.0

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Mo S Kr

16 32 1

Direct

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0.8335888337896904 0.1664111662422769 0.4195720769282971
0.8336377804174333 0.4163828307782040 0.5804395964428863
0.8335898749992197 0.4163914611160280 0.4195720613121239
0.8335556185644819 0.6663328277867748 0.5804021040866232
0.8336641045072994 0.6664364782250303 0.4195299163711681
0.8335531796226974 0.9163287001842519 0.5804022827827495
0.8336620286383791 0.9164393678575706 0.4195302287773899
0.4168956945344391 0.5831043049962261 0.7595033962507665

Ti-MoS_2@H

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Mo S Ti
16 32 1
Direct
0.1663615142678828 0.0824973673858851 0.4994408033890539
0.1633525791266633 0.3312586363610304 0.4997866687599488
0.1663623233703852 0.5830322610393233 0.4994409726187573
0.1669437396387186 0.8330559321598157 0.4991807315624045
0.4169673796957987 0.0824967539968337 0.4994407254572068
0.4181176559861371 0.3353997199678265 0.5016943740587088
0.4181179427038951 0.5818818071763365 0.5016942140995321
0.4169674793330344 0.8336374294768024 0.4994409976799987
0.6672609703498050 0.0832133982710112 0.4986322349291879
0.6687415354239953 0.3312581894191324 0.4997872497200123
0.6645999983955024 0.5818820783990366 0.5016944105995503
0.6687411567486458 0.8366472875235008 0.4997867201975867

0.9167854446255739 0.0832143841476432 0.4986320142679663
0.9167863942084700 0.3327387918577457 0.4986322216615039
0.9175029328172158 0.5830323237945110 0.4994407260392081
0.9175023324454363 0.8336382167645697 0.4994408242314577
0.0811133342080377 0.1639186584172002 0.5801533379182697
0.0840555315193097 0.1661627191433993 0.4182459288547788
0.0811151356135215 0.4163622847441270 0.5801531312575783
0.0840567782613972 0.4170590943575881 0.4182463429923423
0.0839512796848315 0.6670708679411600 0.5803064932993228
0.0835176047351758 0.6662004108769981 0.4183190066659052
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0.0835169452951054 0.9164832413550550 0.4183190074933937
0.3330350689839365 0.1652382787057985 0.5803270687601624
0.3350573159707200 0.1692808704171702 0.4201090897574086
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Ni-MoS_2@T_{Mo}

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Mo S Ni

16 32 1

Direct

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0.1669523426390849 0.8330476573607825 0.4995569464086347

0.4168427972571602 0.0830053244273435 0.4994694981055979

0.4174401458388512 0.3325865899060294 0.5000201471796041

0.4169434460758869 0.5830565539233621 0.4997042058829003

0.4174382361246690 0.8340209153974225 0.5000173237604132

0.6670055470773891 0.0831783341637316 0.4998603002028384

0.6670061011345251 0.3329938988654095 0.4998611216984681

0.6674134100940347 0.5825598541612129 0.5000201471795935

0.6674130060316482 0.8340185574644974 0.5000191504606200

0.9169951567863993 0.0830048432134628 0.4994697099474950

0.9168216658362024 0.3329944529225449 0.4998603002028325

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0.9169265140525114 0.8330469984372408 0.4995581724216634

0.0829139490431266 0.1655579537703377 0.5802257538884010
0.0837538110552180 0.1665884018849312 0.4189678893389803
0.0831780220587715 0.4161755914745464 0.5805469921101312
0.0835589084055385 0.4163586130875341 0.4193366781262758
0.0829134492552226 0.6665287566299162 0.5802247134266576
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0.0836095615182130 0.9163904384778341 0.5800815252717296
0.0836125070186953 0.9163874929849161 0.4189765748609021
0.3334721058657356 0.1655570886332476 0.5802261268013994
0.3336755353787074 0.1665891161400500 0.4189681609982835
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0.3339275038293863 0.4170119019612976 0.4201666691901724
0.3304411390803141 0.6695588609157930 0.5833113207796403
0.3339263820444389 0.6660736179597742 0.4201649833612098
0.3334712433662065 0.9170865507408998 0.5802247134266623
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Kr-Ti-MoS_2@H

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Mo S Ti Kr

16 32 1 1

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0.9167800304024709 0.0832240015457302 0.4984324401508076

0.9167769990442238 0.3327302369282776 0.4984404459565965

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0.9175097913637558 0.8336280235495650 0.4992400243572277

0.0811634905823269 0.1639969860067438 0.5799222376090185

0.0840435072957035 0.1661146571498051 0.4180355701667580

0.0811685596183267 0.4163575279955225 0.5799264313086425

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0.0835446034387459 0.6662498663352636 0.4181481470533939
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0.3338459717919235 0.4164851842186437 0.4213056510586810
0.3331065944363658 0.6669055948452254 0.5801016305213551
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0.3329661229435601 0.9160641843885458 0.5801463860797540
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Kr-Ni-MoS_2@T_{Mo}

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Mo S Ni Kr

16 32 1 1

Direct

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0.4173872306950983 0.3324853289419920 0.5000045116211993

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Xe-Ti-MoS_2@H

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Mo S Ti Xe

16 32 1 1

Direct

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0.8338279585300157 0.9159403600321880 0.4182593352734898
0.5001170272155733 0.4998124587565087 0.6364701150253111
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Xe-Ni-MoS$_2$@T$_{Mo}$
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-6.3129143705171531 10.932783493509 4 -0.0001652248573488
0.0003508277494425 -0.0000905615859908 19.4099298153827107
Mo S Ni Xe

16 32 1 1

Direct

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The reader may request to the authors for other remaining structure files in this work.

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