

Incorporation of oxygen atoms as a mechanism for photoluminescence enhancement of chemically treated MoS₂

*Christian Schwermann^a, Torsten Stiehm^b, Philipp Tonndorf^b, Robert Schneider^b, Robert Schmidt^b, Johannes Kern^b, Steffen Michaelis de Vasconcellos^b, Rudolf Bratschitsch^b and Nikos L. Doltsinis *^a*

^aInstitute of Solid State Theory and Center for Multiscale Theory and Computation,
Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster,
Germany

^bInstitute of Physics and Center for Nanotechnology,
Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster,
Germany

*E-mail: nikos.doltsinis@wwu.de

Supporting Information

Table of Contents

1. Implementation of Grimme's D3 model in CPMD	2
2. Results and discussion	4
2.1 Reaction barriers	4
2.2 MoSe ₂ band structure	7
2.3 Reaction of O ₂ with MoS ₂	8
2.4 Structural parameters	10
2.4.1 XYZ coordinates of initial, transition and final state structures	11
References	42

1. Implementation of Grimme's D3 model in CPMD

The Implementation of Grimme's D3 model in CPMD was tested on the S22 set of non-covalently bound molecules.¹ For comparison the geometries were optimized with the ORCA 4.0.0 package² using either D3 dispersion with zero damping (D3-Zero) or with Becke-Johnson damping (D3-BJ). The calculations were performed with the BLYP functional^{3,4} and the reference calculations employed the def2-TZVP basis set of Ahlrichs and coworkers.^{5,6}

Figures S1 and S2 show only negligible deviations of the CPMD results from the Orca results, confirming the correctness of our implementation. Table S1 further shows acceptable mean and maximum energy deviations as well as small mean Root Mean Squared Distance (RMSD) deviations, while the maximum RMSD deviation of 0.1785 Å and 0.1746 Å respectively for Complex 18 can be explained by the different basis sets employed in the calculations. Complex 18 contains a hydrogen bond and thus the interaction of the molecular orbitals gives a significant contribution to the corresponding bond length.

Table S1. Mean and maximum RMSD as well as mean and maximum absolute energy deviations of geometries from CPMD calculations w.r.t. Orca results.

	D3-Zero	D3-BJ
RMSD / Å	0.0504	0.0496
RMSD _{max} / Å	0.1785	0.1746
ΔE _{disp} / eV	0.0102	0.0062
ΔE _{disp} _{max} / eV	0.0261	0.0414

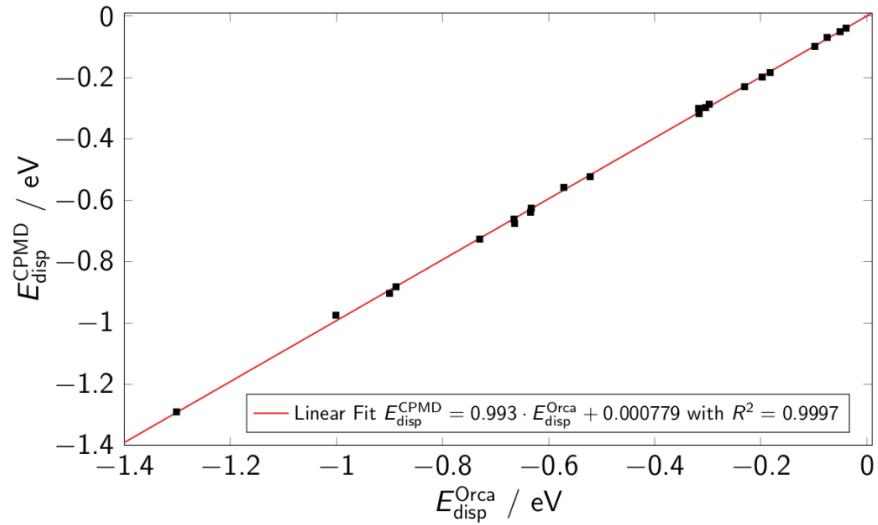


Figure S1. Comparison of dispersion energies for the S22 set obtained with the D3-Zero model in Orca and CPMD respectively.

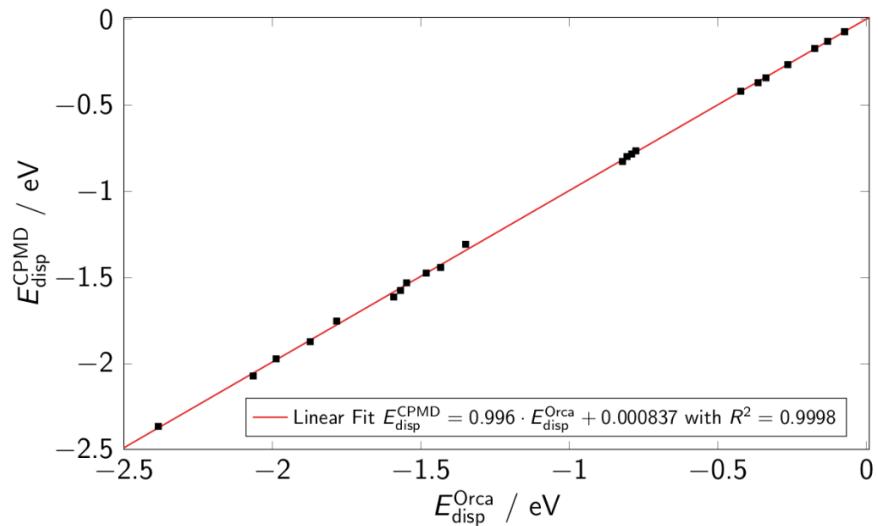


Figure S2. Comparison of dispersion energies for the S22 set obtained with the D3-BJ model in Orca and CPMD respectively.

2. Results and discussion

2.1 Reaction barriers

Figure S3 shows the initial, transition state and final structures of TFSI, H₂O₂, H₂SO₄ and H₂O, corresponding to the minimum at high ξ , the position of the barrier and the minimum at low ξ respectively, as portrayed in Figure 1. Section 2.4 summarizes the corresponding structural parameters. We note that for water there is no clear transition state, as the reaction has no clearly discernible barrier.

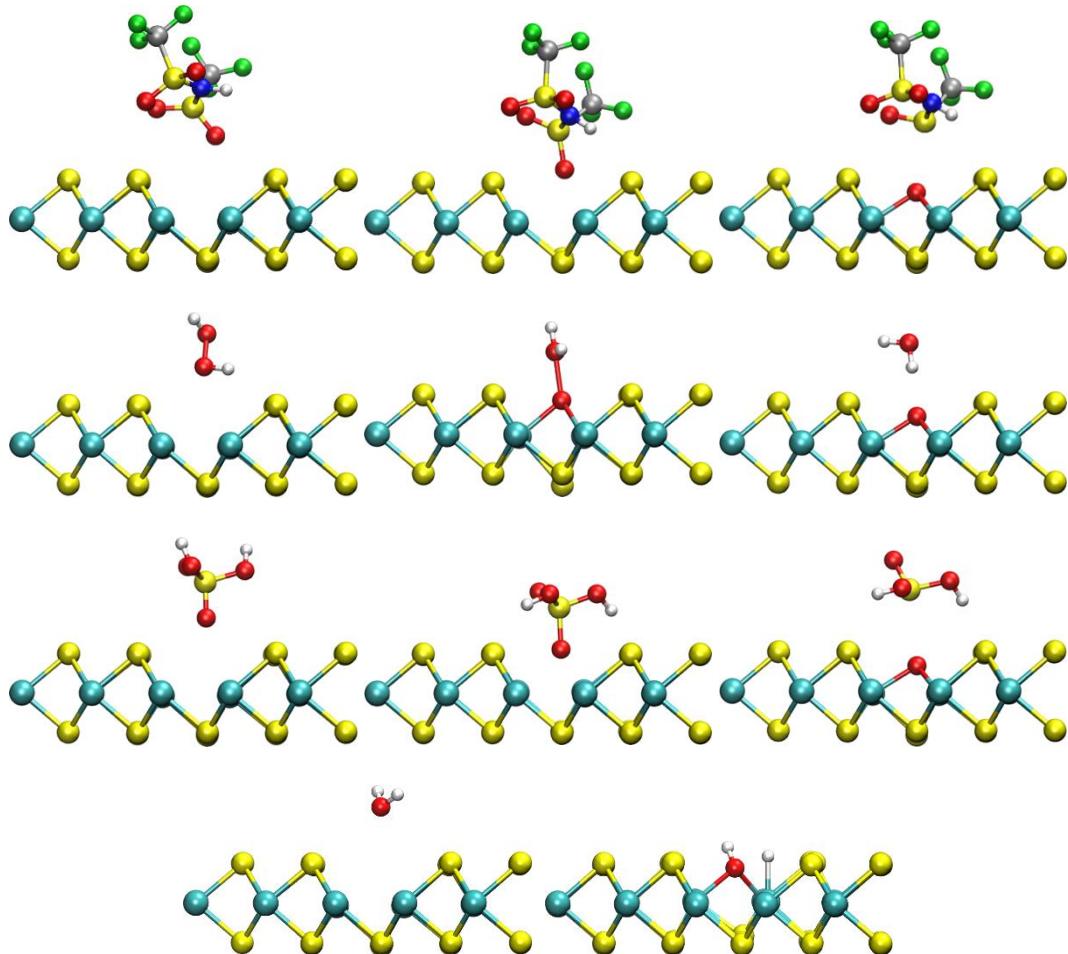


Figure S3. Initial, transition state and final structures for the oxygen transfer reaction from TFSI, H₂O₂, H₂SO₄ and H₂O to defective MoS₂.

A comparison of the potential energy landscapes for the oxygen transfer reaction from TFSI to defective MoS₂ and MoSe₂ is presented in Figure S4 with the corresponding structures for MoSe₂ being shown in Figure S5. The higher reaction barrier as well as the position of the barrier being shifted to higher ξ observed for MoSe₂ can be attributed to the larger van-der-Waals radius of selenium compared to sulfur, i.e. 1.771 Å for selenium and 1.683 Å for sulfur

in Grimme's DFT-D2 model⁷ (in the DFT-D3 model there is no unique van-der-Waals radius defined, though the effect should be similar).

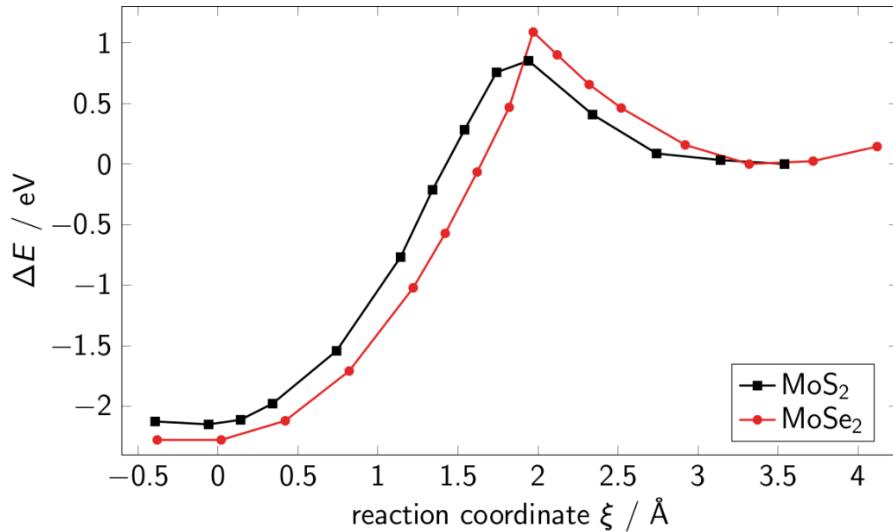


Figure S4. Barriers for the oxygen transfer reaction from TFSI to defective MoS₂ and MoSe₂ respectively.

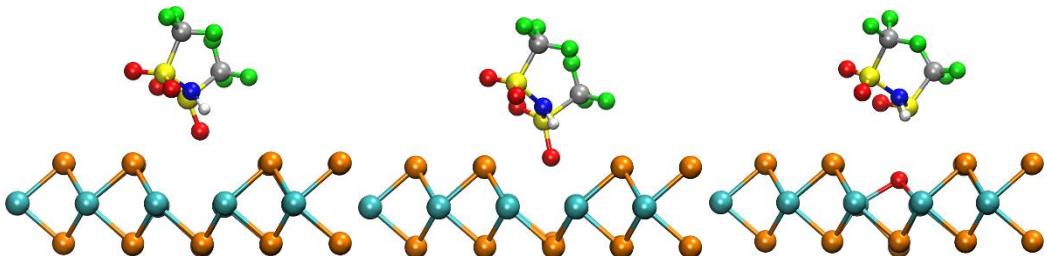


Figure S5. Initial, transition state and final structures for the oxygen transfer reaction from TFSI to defective MoSe₂.

Since explicit inclusion of solvent molecules is computationally prohibitive and there is currently no implementation of continuum solvation models available in the CPMD package, we conducted calculations of deprotonated TFSI (denoted as TFSI⁻) on MoS₂ and MoSe₂ (see Fig. S6). As deprotonation is supposed to be the most prominent feature of acids in solution, these calculations should approximately demonstrate the changes expected from solution phase calculations. As deprotonation results in negatively charged systems, a positive background charge is included in the computations to yield a finite total energy. However, interactions between periodic images cannot be eliminated completely.

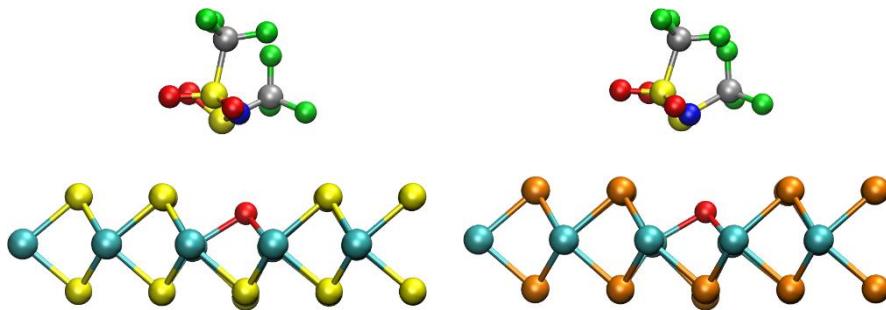


Figure S6. Final structures of deprotonated TFSI on defective MoS₂ and MoSe₂.

The resulting potential landscapes of the anionic species is shown in Figure S7. For both systems, the reaction barrier is lower than for the corresponding neutral systems (see Tab. S2). While the difference in barrier heights compared to the neutral systems - 0.17 eV and 0.18 eV respectively - is not insignificant, it is approximately the same for both MoS₂ and MoSe₂, resulting in the same trend for the respective reactivities. Based on these two systems we infer that the trends obtained for the other molecules as shown in Fig. 1 and Tab. 1 remain qualitatively unchanged in solution.

Table S2. Activation barriers $\Delta E^\#$ and reaction energies ΔE together with reaction temperatures T assuming a reaction rate of 1 s^{-1} estimated by Transition State Theory.

System	$\Delta E^\# / \text{eV}$	T / K	$\Delta E / \text{eV}$
MoS ₂ +TFSI	0.853	335	2.145
MoSe ₂ +TFSI	1.090	763	2.273
MoS ₂ +TFSI ⁻	0.683	270	1.715
MoSe ₂ +TFSI ⁻	0.908	356	1.898

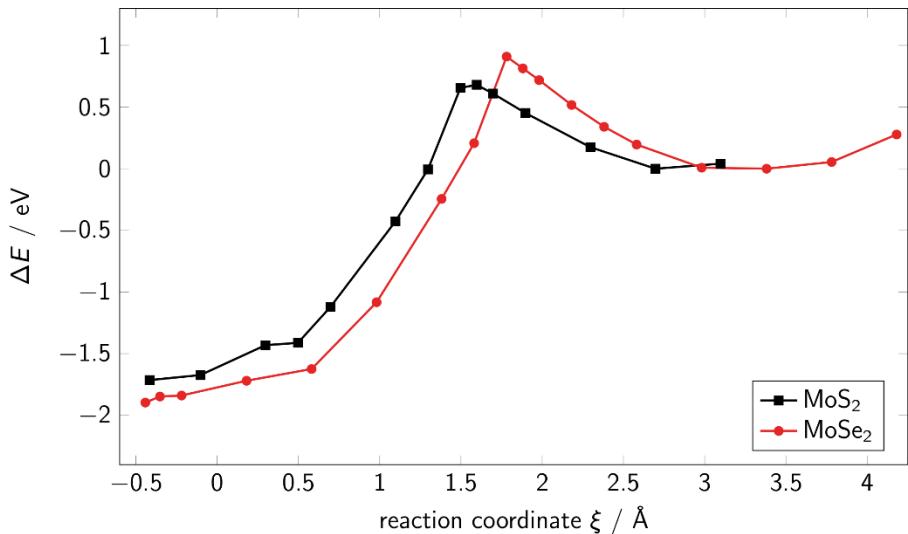


Figure S7. Barriers for the oxygen transfer reaction from deprotonated TFSI to defective MoS₂ and MoSe₂.

2.2 MoSe₂ band structure

While the reaction barrier for the insertion of oxygen into defective MoSe₂ is higher than for MoS₂ (see Fig.S4), the effects on the band structure are similar. The defect band induced by a selenium vacancy (Fig. S8 bottom row, middle) vanishes upon incorporation of an oxygen atom.

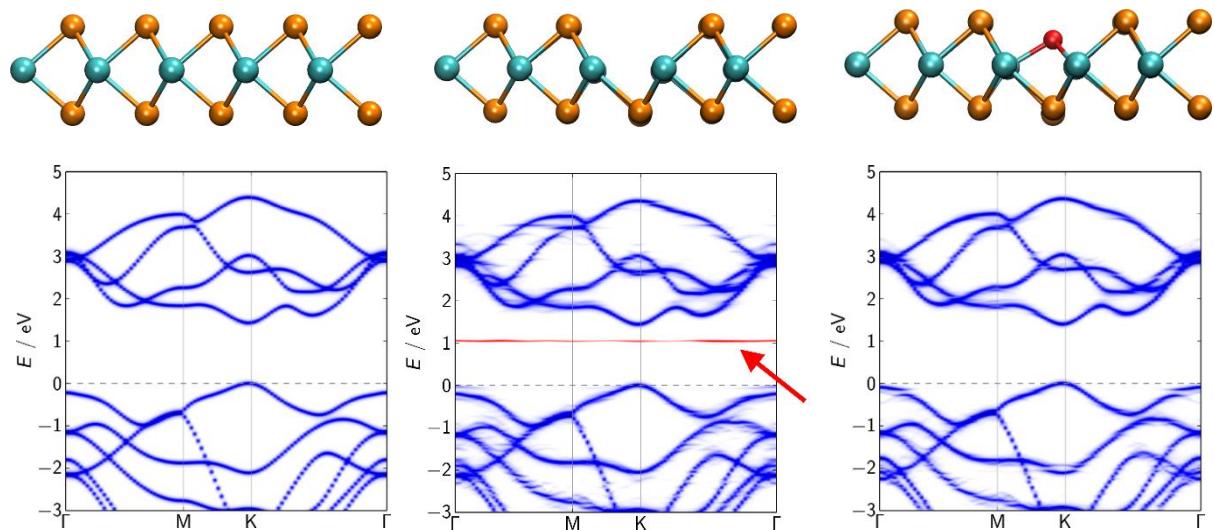


Figure S8. Geometric unit cell structures (top row) and electronic band structures (bottom row) of pristine MoSe₂ (left), MoSe₂ with a selenium vacancy (middle), and MoSe₂ with a selenium vacancy filled with an oxygen atom (right).

2.3 Reaction of O₂ with MoS₂

As the ground state of O₂ is a spin triplet, the whole system was described using the ROKS method⁸ for triplet states. However, around $\xi = 2.64 \text{ \AA}$, the singlet state becomes the energetically lowest configuration, according to spin-restricted calculations. Fig. S9 shows the corresponding energies for the reaction paths, Fig. S10 shows the initial, transition state and final (in the S₀ state) structures.

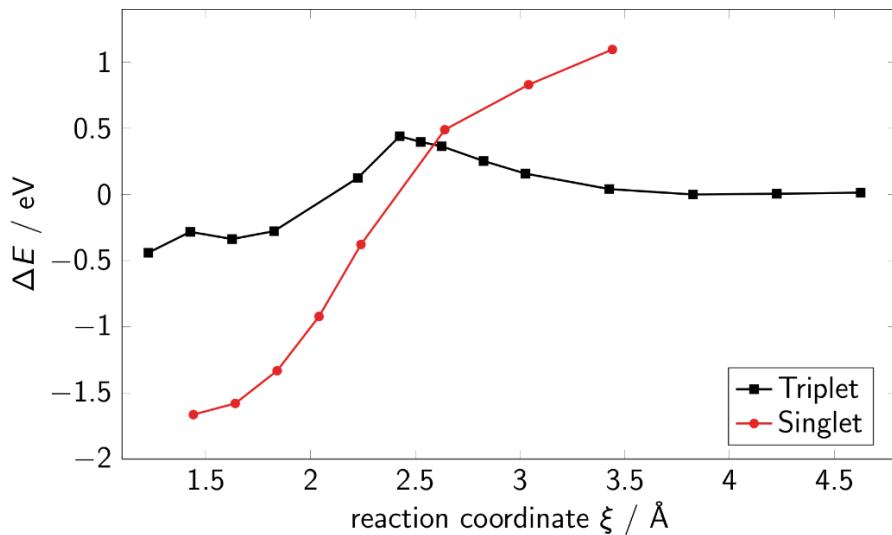


Figure S9. Barriers for the chemisorption of O₂ on defective MoS₂ calculated for the spin-restricted singlet stage and the ROKS triplet state.

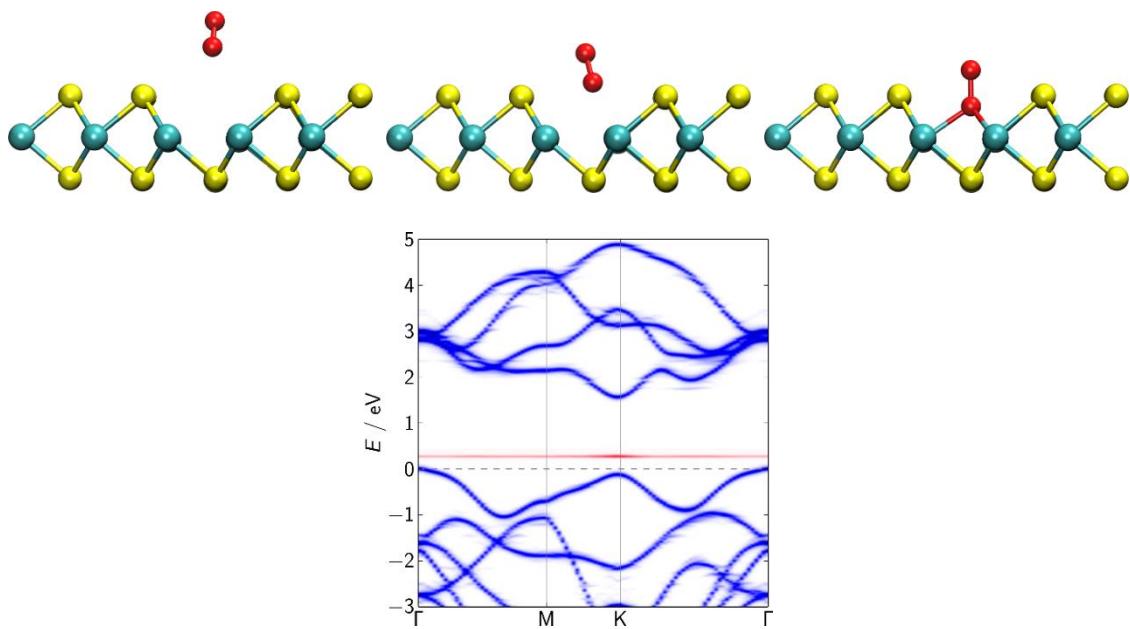


Figure S10. Optimized initial (top left), transition state (top middle), and final (top right) structures of the oxidation reaction of defective MoS₂ with O₂ as well as electronic band structure for the final state (bottom).

As literature reports indicate different barrier heights,^{9–11} reference calculations employing the spin-unrestricted Kohn-Sham formalism, the Grimme-D2 dispersion correction,⁷ no additional dispersion correction, the LDA^{12,13} and BLYP^{3,4} density functionals, as well as the optB88-vdw non-local density functional¹⁴ were performed. The latter calculations were done using the climbing-image nudged elastic band (CI-NEB) method^{15,16} as implemented in GPAW^{17–19} at the Γ point in the unrestricted Kohn-Sham formalism and with a $4\times4\times1$ k-point mesh and a double-zeta polarized basis set.²⁰ Ionic forces below 0.05 eV/Å were considered converged. The resulting barrier heights are summarized in Table S3.

Table S3. Activation barriers $\Delta E^\#$ for chemisorption of O₂ on defective MoS₂ calculated with different methods. ‘RO-’ denotes use of ROKS, while ‘U-’ indicates the unrestricted Kohn-Sham formalism. D2 and D3 denote the corresponding Grimme dispersion corrections.

Method	$\Delta E^\# / \text{eV}$
RO-PBE-D3	0.40056
U-PBE-D3	0.40029
RO-PBE-D2	0.39981
RO-PBE	0.56296
U-LDA-D3	0.40029
U-BLYP-D3	0.37561
optB88-vdW (Γ point)	0.38740
optB88-vdW ($4\times4\times1$)	0.38743

The final structure with only one oxygen atom bound to Mo atoms (see Fig. S10) corresponds to the most stable structure reported by Gogoi et al.,¹⁰ but we found a structure with both oxygen atoms bound to Mo atoms, as reported by Liu et al.,¹¹ to be more stable by 0.18 eV. While the configuration with only one oxygen atom bound to an Mo atom exhibits a flat defect band (see Fig. S11c), potentially enabling non-radiative processes, the more stable structure with both oxygen atoms partaking in bonds to Mo atoms recovers the band structure of pristine MoS₂ (see Fig. S11d).

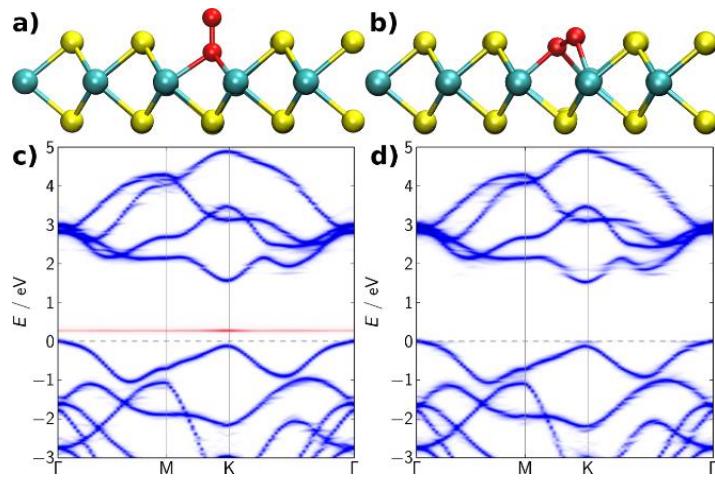


Figure S11. Product configuration of the chemisorption reaction of O_2 on MoS_2 with the molecular axis pointing perpendicular to the surface (a) with corresponding band structure (c, defect band is highlighted red) and more stable structure with both O atoms incorporated (b) with corresponding band structure (d).

2.4 Structural parameters

Table S4. Reaction coordinate ξ and contributing distances r_{12} and r_{23} for the initial, transition and final states of the oxidation reaction of various compounds on MoS_2 as well as TFSI on $MoSe_2$.

Compound	State	$\xi / \text{\AA}$	$r_{12} / \text{\AA}$	$r_{23} / \text{\AA}$
TFSI	initial	3.541	4.989	1.448
	transition	1.941	3.508	1.567
	final	-0.059	2.779	2.838
H_2O_2	initial	3.198	4.735	1.537
	transition	1.398	3.354	1.956
	final	-0.202	2.750	2.952
H_2SO_4	initial	3.211	4.650	1.439
	transition	1.611	3.285	1.674
	final	-0.357	2.754	3.111
H_2O	initial	4.480	5.470	0.990
	final	1.480	3.130	1.650
O_2	initial	3.826	5.067	1.241
	transition	2.426	3.695	1.269
	final	1.441	2.806	1.365
TFSI+ $MoSe_2$	initial	3.321	4.779	1.458
	transition	1.974	3.570	1.596
	final	-0.321	2.866	3.187
TFSI ⁻	initial	2.697	4.190	1.493
	transition	1.597	3.339	1.742
	final	-0.416	2.758	3.174
TFSI ⁻ + $MoSe_2$	initial	3.381	4.852	1.471
	transition	1.781	3.495	1.714
	final	-0.442	2.855	3.277

2.4.1 XYZ coordinates of initial, transition and final state structures

	77		
H2O	initial		
H	9.635323622685	8.190479606964	13.605096343245
H	8.291408390124	8.944005401353	13.726826859254
O	8.787022557317	8.341451755725	13.117019993368
S	10.321852457733	5.723604376314	10.836510272670
S	7.175899418741	5.656552347411	7.703262842463
S	7.242020985995	5.724017107864	10.836774386592
S	11.967445868325	2.894065927801	7.761035319457
S	5.597859561059	2.893913938570	7.760332713023
S	7.240654322508	11.061492779034	10.836374041155
S	10.324186246424	11.062521461438	10.836545022535
S	11.864873352153	8.394936093994	10.836804995172
S	7.215341019228	11.153256748049	7.704574126520
S	5.611802956208	13.878158625482	10.888990624030
S	5.612128020781	13.901689942797	7.761256189168
S	8.782911726360	13.874471104915	10.892098666183
S	8.782324613880	13.904397737775	7.764212623496
S	10.349938795260	11.153291868780	7.704120159328
S	11.953205446283	13.878378472676	10.888558767314
S	11.953315881533	13.901679735048	7.760664743273
S	11.956752650882	8.370926568919	7.705092157470
S	13.514401322867	11.125944462498	10.862481254050
S	13.548417329722	11.145175942510	7.744816025547
S	13.529178290943	5.652803073692	10.892377526278
S	13.555323754086	5.638346960064	7.764594337907
S	15.117998254018	8.397224165758	10.889456333021
S	15.138240797717	8.385098625390	7.761461964042
S	15.132709781764	2.887608384815	10.906638989372
S	15.140053466045	2.892123160571	7.778314769221
S	16.726335668900	5.647065354208	10.906738996343
S	16.725902924253	5.638861263546	7.778397487875
S	18.319506661790	2.887799107717	10.906243629825
S	18.311535350055	2.892186202616	7.777909988558
S	11.946687530496	2.905900098539	10.888933355806
S	10.388949578746	5.656475910058	7.704196851800
S	8.782450664628	8.392964301618	7.647370539640
S	5.700898054330	8.394292146513	10.836712575427
S	5.608703336717	8.370435055248	7.704321780784
S	4.050585990427	11.125326165917	10.861982020469
S	4.016340169240	11.145106295746	7.744618101163
S	2.430208856465	13.898787915733	10.879938936231
S	2.430661843143	13.898884090355	7.756286840593
S	-0.752072512301	13.898636842184	7.756023117876
S	0.839213400054	11.142456270425	10.880070980781
S	0.839069652163	11.141884968591	7.756279784493
S	-0.751792280684	13.898749790595	10.879984542742
S	2.447862534933	8.397188017405	10.889259114076
S	2.427239972718	8.385044975394	7.761210458801
S	4.036695065703	5.652912600038	10.892038491798
S	4.010008461090	5.638576522641	7.763848575792
S	5.618313765883	2.906144862497	10.888433946185
S	8.781999115989	2.930471286360	10.862191755765
S	8.782316403357	2.890876691661	7.744257811875
Mo	8.781863077736	4.762614690180	9.273755922277
Mo	7.193756614082	1.981335118740	9.317309563079
Mo	10.371041991075	1.981745580552	9.317472650330
Mo	11.950305710985	4.739927088960	9.315465259745
Mo	10.323386247868	7.503607760296	9.224991365001
Mo	8.783018408866	10.172636156635	9.225120181790
Mo	5.637534133304	10.208899149505	9.273823072538
Mo	2.434458449109	10.223714061260	9.317749656967
Mo	4.034411980745	7.476947031530	9.316015184140
Mo	7.241187197615	7.502866456935	9.225648183992

Mo	5.615040708869	4.740073627592	9.314859209888
Mo	13.547777988179	1.973009339859	9.334913218733
Mo	16.725924975462	1.969769916283	9.341772321349
Mo	15.134364342767	4.726471977478	9.342038656212
Mo	13.531366163516	7.476973267633	9.316132925506
Mo	11.927468604723	10.209795648005	9.274318840114
Mo	10.362989669731	12.963979470926	9.315141282279
Mo	7.202274144366	12.964009675635	9.315884289207
Mo	4.023437624033	12.975956471878	9.317608374928
Mo	0.839089504838	12.979794943646	9.317683101879
Mo	-2.344535371976	12.975979939684	9.317513365452
Mo	-0.756062625296	10.223850425885	9.317870531537
Mo	0.839678285705	7.477187630293	9.335339213660
Mo	2.431440344012	4.726575164892	9.341697967084
Mo	4.017530179332	1.973047724326	9.334295330935

77

H2O transition

H	9.694599478238	7.871676667634	10.619770186095
H	7.704672395701	9.021816520046	11.745912107883
O	8.309534795418	8.672718902348	11.024765572978
S	10.449280077709	5.633559540469	10.902771811947
S	7.205820112208	5.705525410401	7.900646815406
S	7.251413594804	5.656272828662	11.006964679300
S	11.985008524953	2.843393438016	7.782652347809
S	5.626103926615	2.901695427717	7.872030723540
S	7.144537349014	11.207417902899	10.989942549422
S	10.392074803012	11.096281455433	11.006838476849
S	12.010465645673	8.337910212985	10.902765605042
S	7.234034856927	11.128687521710	7.872155144366
S	5.602409604817	13.913029978292	10.949585983485
S	5.631178429827	13.875536404400	7.811869741069
S	8.790169411646	13.900765500703	10.984136534691
S	8.821804114054	13.871356670793	7.852600883944
S	10.326777758176	11.111104646856	7.900425416767
S	11.982509123654	13.883695502633	10.996909033766
S	11.965058446470	13.880965097977	7.871919268060
S	12.054001514424	8.436567271297	7.740210543950
S	13.573557325716	11.116428655030	10.960312243042
S	13.549793756419	11.154097303104	7.840482804553
S	13.578688546030	5.629671170273	10.891326250438
S	13.596446744291	5.619475341444	7.769468182914
S	15.160583776067	8.375319753077	10.923575931384
S	15.194864003614	8.403023606136	7.782757541669
S	15.149943921471	2.892327748096	10.935224416137
S	15.182445470280	2.860864518777	7.804388042062
S	16.734912326299	5.637658457703	10.935290756146
S	16.778480718813	5.625339866768	7.804462280698
S	18.326356371860	2.888629136547	10.976481115627
S	18.354209936232	2.872632255009	7.845807726003
S	11.991912295235	2.886877289892	10.923485164272
S	10.385509449301	5.546625971468	7.740188031858
S	8.807808157257	8.384436672042	7.947953218501
S	5.531558210492	8.413179935596	10.990119616571
S	5.644421191424	8.374827273874	7.872411346197
S	4.005542970261	11.156811860769	10.957096162179
S	4.032835296648	11.140964156836	7.814616109357
S	2.446705024151	13.897646097707	10.947395947159
S	2.434562181031	13.888355251505	7.814054901169
S	-0.747445984340	13.900900693566	7.846728517994
S	0.852436285201	11.136364365089	10.947449664383
S	0.854409372763	11.151442970722	7.814097549915
S	-0.721414993534	13.885862581945	10.977582854844
S	2.417041141700	8.395780345006	10.949734659503
S	2.464006518929	8.389491864651	7.812084334987
S	4.021495690633	5.641175540584	10.984328364403
S	4.062856468071	5.628614187475	7.852810490194

S	5.632459318189	2.885051614235	10.996939095338
S	8.824518714732	2.890737401701	10.960308478378
S	8.779931244518	2.892538987947	7.840455812447
Mo	8.817093884514	4.733315358939	9.401486757381
Mo	7.213712107006	1.970424591065	9.420437434581
Mo	10.393891526653	1.964780117915	9.374945117319
Mo	11.997138632136	4.685619892142	9.325461437983
Mo	10.540658586999	7.383616137885	9.269465143879
Mo	8.741851597603	10.214837486741	9.501851707196
Mo	5.596060524273	10.238549762263	9.404037060519
Mo	2.440091327455	10.227278250934	9.379731853398
Mo	4.017511305120	7.471589799395	9.406795682943
Mo	7.189921450149	7.526284298911	9.502026225722
Mo	5.637792209462	4.734321901835	9.446448613203
Mo	13.573146355183	1.959621840969	9.363542821292
Mo	16.752771569593	1.960553879189	9.400836918921
Mo	15.173063004219	4.709205884256	9.350936102187
Mo	13.605464860957	7.471410270609	9.325526170131
Mo	11.974140463110	10.201593836971	9.401469294815
Mo	10.383746323046	12.954563834391	9.446264271192
Mo	7.202961209295	12.989206047224	9.406516046689
Mo	4.027792809053	12.977260573051	9.379638901374
Mo	0.853947349376	12.976336672057	9.391359429776
Mo	-2.321080816683	12.971591873689	9.420413694786
Mo	-0.726121550464	10.220288991879	9.375017828953
Mo	0.868018410560	7.469596817939	9.363688055096
Mo	2.457027134850	4.715513839190	9.400937219464
Mo	4.038713655876	1.965684907107	9.430650478526

77

H2O	final		
H	10.571455186036	7.364593772150	11.257387861241
H	7.786289600784	8.975273590297	11.612984031970
O	8.291559602696	8.683464218421	10.800960810125
S	10.456740707645	5.511622738637	10.995849345354
S	7.209270250687	5.696388995612	7.899691031138
S	7.216569355916	5.662433386918	11.018651194612
S	11.969774567601	2.867360646366	7.780875132081
S	5.617737573867	2.909444702055	7.856184377886
S	7.109846840434	11.225440498089	10.976973892599
S	10.369695108915	11.124070740493	11.018569196831
S	12.120060638928	8.393028763973	10.995650970596
S	7.217374492499	11.145404731366	7.830394498454
S	5.586781430312	13.912798615444	10.920967589956
S	5.616624712104	13.890854608703	7.777726935505
S	8.769529970760	13.910613367280	10.958263506328
S	8.815175461324	13.875533794324	7.830616689925
S	10.336743321798	11.113385473498	7.899510436638
S	11.969349576444	13.898398525360	10.983140662266
S	11.954542369192	13.885035098015	7.856143287939
S	12.002057574214	8.404628541449	7.845540248429
S	13.587229486363	11.148141087816	10.968250620776
S	13.519728396973	11.146901522417	7.847172607624
S	13.603781663639	5.615654908430	10.916536428883
S	13.578395304551	5.630321992017	7.789125645246
S	15.191641200982	8.391686983691	10.926347767954
S	15.166867663963	8.404882805894	7.780905198607
S	15.147433486343	2.886375907041	10.916503829197
S	15.171258156176	2.872306742025	7.784227069215
S	16.739227336941	5.643448021072	10.916506287216
S	16.763355539289	5.629859574648	7.784250136552
S	18.314670548876	2.895826809686	10.951217879807
S	18.346693115203	2.877375010786	7.819558087618
S	11.993590572281	2.852441161446	10.926379608689
S	10.387736038853	5.608179039810	7.845548259717
S	8.851459257684	8.359604232257	8.120937929451
S	5.498906397019	8.434833706350	10.977110877434

S	5.621937495212	8.381598320765	7.830569176067
S	3.990037993025	11.166159626186	10.917639943908
S	4.015474724517	11.151441717305	7.777382677966
S	2.436343425349	13.892900145642	10.923668881320
S	2.415179462738	13.906795495320	7.788429502767
S	-0.766143972489	13.912137453956	7.828639988003
S	0.851740729872	11.148307177014	10.923678143300
S	0.829136283615	11.159658616624	7.788452093698
S	-0.729864964500	13.891187628271	10.961775250744
S	2.409808588664	8.409995326744	10.921018366955
S	2.443833340646	8.395070942692	7.777816047644
S	4.003078837501	5.654769492982	10.958344314734
S	4.056340020207	5.632854929832	7.830727279863
S	5.613563412200	2.889845135656	10.983159440921
S	8.804240077835	2.863687695342	10.968247943359
S	8.771554249387	2.922805910618	7.847152825445
Mo	8.800977529102	4.730098329673	9.446820632610
Mo	7.199935505700	1.975716468387	9.409417316401
Mo	10.381443421002	1.968302905763	9.366211071933
Mo	12.004779177915	4.674047389815	9.359643968705
Mo	10.559533392336	7.373088179323	9.466326087603
Mo	8.709573083946	10.275792317626	9.484324920527
Mo	5.579616445329	10.248473347359	9.368356507253
Mo	2.424395917607	10.235583478947	9.344150247561
Mo	3.999126231435	7.485004990371	9.374964072915
Mo	7.121335235072	7.524431603168	9.484549337047
Mo	5.625099061444	4.738943382654	9.434872868020
Mo	13.564695277072	1.961807491894	9.343101040398
Mo	16.743802627649	1.966510218576	9.374625615370
Mo	15.170291384632	4.711229293535	9.344326345678
Mo	13.619634497556	7.471228440553	9.359608572498
Mo	11.969197250499	10.217907230561	9.446794508623
Mo	10.373755544841	12.963958072523	9.434771513650
Mo	7.182492423433	12.999048262049	9.374817075122
Mo	4.013088092608	12.987329431590	9.344120637273
Mo	0.839673872916	12.985011646610	9.365686387442
Mo	-2.332158865795	12.981540209374	9.409416821794
Mo	-0.735026201298	10.229947529703	9.366231444619
Mo	0.862291331854	7.476422089557	9.343122740500
Mo	2.447780026906	4.720924123280	9.374656764179
Mo	4.028141621481	1.972264415594	9.409953186168

78

H2O2 initial

H	8.224023823695	8.317980887819	14.343224264156
H	9.635048763742	8.567502761515	12.351544458403
O	8.662892718115	8.344661148636	12.446264234930
O	8.351117858483	9.105488922343	13.745033843276
S	10.328822934741	5.710896661881	10.871357950734
S	7.179347035644	5.662600971919	7.753362618778
S	7.238582333884	5.706793967108	10.875176854165
S	11.969425539718	2.892647445516	7.795305277945
S	5.600580916196	2.894181183093	7.795672727522
S	7.239769806892	11.073834895781	10.872744056927
S	10.336705673410	11.076003628578	10.874216814099
S	11.876678368622	8.399024240837	10.874217858788
S	7.223454463103	11.147579442005	7.753641142180
S	5.613135555818	13.880265816535	10.914381066936
S	5.614824642580	13.899288453520	7.796273503186
S	8.783764562873	13.881048438517	10.917991697846
S	8.784875578881	13.902786150538	7.799354962675
S	10.347696488261	11.150707419451	7.752790954554
S	11.957572356033	13.882374106811	10.914165887009
S	11.954080645250	13.900676633939	7.796352758409
S	11.957105532584	8.370888059615	7.751952244096
S	13.521920065741	11.129675391897	10.889957306396
S	13.549150002219	11.143973665340	7.782170575990

S	13.535481914601	5.647695819615	10.917667942993
S	13.556454922534	5.639603347906	7.800382000248
S	15.124030883682	8.396913894963	10.915612243366
S	15.139171060584	8.384067748069	7.798408651434
S	15.135742281045	2.887845367429	10.927688643141
S	15.141493284815	2.891764205371	7.809733317257
S	16.728599192672	5.645161126709	10.928742782433
S	16.728325691925	5.640182188456	7.810518547995
S	18.320167986128	2.888487470714	10.927642133857
S	18.314415443110	2.892084448342	7.809368955295
S	11.950417574027	2.901776852016	10.913022974331
S	10.389070902705	5.656844276167	7.748664617432
S	8.783759673030	8.392338175634	7.712830737221
S	5.690154100955	8.391829681599	10.874046994978
S	5.620166471264	8.367238606590	7.755974469965
S	4.051075987436	11.126929273339	10.892113780279
S	4.024762376856	11.141092107876	7.784489688731
S	2.432915991326	13.896845424869	10.904410009094
S	2.434062483559	13.896023038566	7.791009825724
S	-0.749493898592	13.897194493271	7.790617448599
S	0.842513760937	11.142350232242	10.905351835377
S	0.842963463697	11.140359827048	7.792067594049
S	-0.748829934781	13.897464006604	10.904368521192
S	2.447777983179	8.396940482937	10.915697102806
S	2.431364582804	8.385395463116	7.797679591389
S	4.034174856713	5.649543882888	10.918075910678
S	4.014195371013	5.639289016824	7.799529770596
S	5.619078035066	2.901538986816	10.913579347449
S	8.784516717708	2.922122512270	10.889296800681
S	8.784436808255	2.891697939495	7.781327592255
Mo	8.783636978528	4.758138083240	9.312354210913
Mo	7.195775045868	1.979427404390	9.346939356174
Mo	10.373953797499	1.979140682654	9.346833259709
Mo	11.954163760470	4.737015572441	9.346670512601
Mo	10.329584300172	7.499349964051	9.271945003762
Mo	8.788764251182	10.174983078558	9.280380922618
Mo	5.641636798349	10.208449683914	9.316023023302
Mo	2.438185342309	10.223398292344	9.349269320838
Mo	4.034727407620	7.475667081194	9.349913849763
Mo	7.244863917913	7.498353450801	9.284055641262
Mo	5.615116287093	4.737251868358	9.348904416816
Mo	13.550319974414	1.972106024361	9.362712558527
Mo	16.728062516935	1.970797193563	9.368217703465
Mo	15.137417243214	4.725971172975	9.368872500732
Mo	13.535677154477	7.475234514523	9.351125089674
Mo	11.931966978197	10.213034055916	9.312129984585
Mo	10.365156170400	12.968097513180	9.350167008099
Mo	7.204521448205	12.966158195984	9.348650160938
Mo	4.026677225143	12.974765802111	9.348401750043
Mo	0.842045370087	12.978638920865	9.347325815603
Mo	-2.342164934191	12.976521237320	9.347515668208
Mo	-0.752929507351	10.223605352874	9.348637300579
Mo	0.842444255536	7.477023348734	9.364822913436
Mo	2.433077063762	4.726295172469	9.368580949483
Mo	4.019403842010	1.973156099722	9.362611569211

78

H2O2 transition

H	8.135028364791	8.678711632152	13.595572127771
H	9.084001474218	7.808439027615	12.730471293083
O	8.791164845052	8.363390911380	10.719419726641
O	8.402490482297	8.520797873570	12.641907206115
S	10.363835780894	5.693445586227	10.897233962105
S	7.226057398479	5.639734460127	7.799729858511
S	7.258215663402	5.693118888945	10.894599417481
S	11.995408027320	2.873150077198	7.830580970720
S	5.635475556946	2.870040062307	7.826306717947

S	7.271688037187	11.052434683941	10.903129499672
S	10.352565881156	11.049734977306	10.906854699419
S	11.905945162397	8.360453601189	10.899941191768
S	7.248617972163	11.107433005451	7.808981992756
S	5.647489184735	13.855667723339	10.943673692798
S	5.646100911589	13.870523057636	7.830196994664
S	8.813602727079	13.854066700498	10.950127665753
S	8.816496123255	13.869562188140	7.825588025001
S	10.380608085509	11.106980863163	7.812390973984
S	11.982941572934	13.857132347926	10.944906819877
S	11.983546477910	13.867129457302	7.832051138426
S	11.973937277756	8.361464347710	7.805724979565
S	13.558551527071	11.108910030915	10.936559691372
S	13.578436793177	11.121759468840	7.815814285756
S	13.564891581369	5.627757304176	10.947982026170
S	13.579279102881	5.618861776797	7.823833592553
S	15.151916988980	8.369614163971	10.942098299511
S	15.162435439430	8.366376124911	7.829682261022
S	15.168538609445	2.865732900857	10.952888020822
S	15.169950170482	2.865926182105	7.837195411368
S	16.760393243082	5.621358223495	10.949589430404
S	16.756453161434	5.618117648601	7.834071748615
S	18.350455824427	2.866624779059	10.950943184572
S	18.346776532434	2.863603550165	7.834505344235
S	11.982733313110	2.881814317458	10.943026253959
S	10.404583986447	5.637508661496	7.803072563331
S	8.818495952610	8.369883821737	7.365078320713
S	5.716495848139	8.357356470066	10.894065792197
S	5.657947990646	8.360812666303	7.799464075130
S	4.071280563380	11.107197738002	10.932284849107
S	4.050032146786	11.122591508828	7.811708244567
S	2.464327842289	13.874963492205	10.939586329090
S	2.463900093165	13.874372248389	7.826902367045
S	-0.720033176829	13.872056767519	7.827254713716
S	0.873198192565	11.117559988943	10.939172171206
S	0.870107069562	11.119346200425	7.826402521223
S	-0.718732032510	13.875360978511	10.939900645848
S	2.481838486045	8.369021091783	10.937312579143
S	2.462895872666	8.367304395521	7.823900486106
S	4.065764191760	5.629346741757	10.940196528149
S	4.048915292281	5.616510309235	7.815617227117
S	5.647348173349	2.884062225720	10.939169466803
S	8.813196923463	2.892653417560	10.931278508749
S	8.814923938438	2.863790955886	7.810268313411
Mo	8.812558401574	4.716377542854	9.350576609175
Mo	7.228114188958	1.956102333655	9.380287236012
Mo	10.401552738864	1.957190031723	9.381780877375
Mo	11.985198253423	4.720342055837	9.379974263241
Mo	10.292072644398	7.514340570303	9.304120819071
Mo	8.812576765266	10.071542335251	9.320374280121
Mo	5.652307079577	10.194531965626	9.354308994061
Mo	2.467932980332	10.202626198684	9.379697978057
Mo	4.069133764447	7.449384026360	9.369713751666
Mo	7.334510771659	7.514486932705	9.307847058433
Mo	5.644197947247	4.719931238771	9.373122951344
Mo	13.581146753223	1.948541496470	9.393115370001
Mo	16.758616056993	1.943432544728	9.393955145498
Mo	15.164665999289	4.704010577096	9.393363234920
Mo	13.559292854178	7.449315222481	9.379596205852
Mo	11.975598072897	10.195855663539	9.359304692424
Mo	10.389106512762	12.937190266081	9.384062740530
Mo	7.240008933467	12.938130660166	9.380345832546
Mo	4.055548366312	12.950452873144	9.382306946843
Mo	0.872621485851	12.955887434513	9.383503043017
Mo	-2.311426906581	12.949892745963	9.384694829302
Mo	-0.725375703483	10.202959679217	9.383384101514
Mo	0.871784487807	7.454013475293	9.389226168204

Mo	2.465166493391	4.703225025758	9.388943594453
Mo	4.049525826345	1.947833871732	9.391174306715

	78		
H2O2	final		
H	7.397462274035	8.279294320585	13.381169079163
H	8.545556898318	8.496915387163	12.363569957312
O	8.840439485079	8.372512663724	10.427816827461
O	8.297952880881	8.685259828791	13.312582722836
S	10.400559772228	5.678803210997	10.919374129860
S	7.240633093731	5.629801349375	7.803201413388
S	7.276935609978	5.678830042471	10.918198898177
S	12.019711016933	2.875668449608	7.831836609135
S	5.657463518526	2.874731750437	7.832090872621
S	7.286277579069	11.077056799551	10.918515853532
S	10.389289307055	11.073813868793	10.919362056197
S	11.952291890153	8.368943033920	10.919210391022
S	7.262276378253	11.129751134318	7.801223425248
S	5.668748750961	13.864784821431	10.946933867681
S	5.666895417211	13.878916234570	7.830246121444
S	8.837377306737	13.863504744340	10.950642127278
S	8.839534332635	13.882046808164	7.829513853528
S	10.414322131423	11.129975792675	7.803288058140
S	12.008649017669	13.864815339179	10.948438617226
S	12.009598551282	13.877873234331	7.832148088851
S	12.013326651197	8.361370762150	7.803569614650
S	13.584203452678	11.114290168698	10.936727960060
S	13.603261258320	11.125274650931	7.819764588065
S	13.592670877207	5.628685631957	10.952098549625
S	13.607739116658	5.620102436034	7.831399170916
S	15.179053197704	8.374335260386	10.948423338230
S	15.189784173943	8.368138088753	7.832277250636
S	15.190646422084	2.868879498963	10.958084330114
S	15.194499390188	2.871943851397	7.838999995665
S	16.781370689711	5.624919688476	10.958247854125
S	16.781101444377	5.620494213521	7.839449150697
S	18.372196280410	2.868896460001	10.958292276647
S	18.369062851098	2.871265221950	7.839178828202
S	12.009131066300	2.881465499625	10.948328369152
S	10.437235876841	5.629811832588	7.803388747130
S	8.839396823743	8.373838480588	7.677697709408
S	5.720824936081	8.368589338513	10.914992410313
S	5.663976276703	8.362006371959	7.803164607917
S	4.092472611311	11.115389696679	10.935845368481
S	4.073575277026	11.125739828654	7.818666698567
S	2.486984014742	13.878088519412	10.943371656848
S	2.486235264450	13.878446587370	7.828401526546
S	-0.695740986899	13.878087688145	7.829105209983
S	0.895835296725	11.122670888633	10.943326701041
S	0.895008676751	11.122906219247	7.828807618467
S	-0.695395860927	13.878016452863	10.943865814586
S	2.497450231758	8.374176967771	10.946964912874
S	2.484946096751	8.368262481217	7.830801004430
S	4.083760679770	5.628749718457	10.950614861672
S	4.068575037111	5.618683857127	7.829793343268
S	5.668458650798	2.881850395487	10.948135372340
S	8.839185352738	2.892153828108	10.936646974986
S	8.838914869161	2.870707460155	7.819514402804
Mo	8.839184797634	4.721791275001	9.363095588733
Mo	7.250581884591	1.959578476084	9.385894662231
Mo	10.427150589166	1.959571663914	9.385624568366
Mo	12.010082112771	4.718315059616	9.385771013337
Mo	10.370473307509	7.489090417866	9.320085652230
Mo	8.837556798306	10.143000333473	9.319913137167
Mo	5.677396059546	10.202005856108	9.362504499947
Mo	2.490044309383	10.205729093003	9.384899003158
Mo	4.085676052134	7.453903644911	9.382964885460

Mo	7.308408114352	7.489582829994	9.318792400194
Mo	5.666707348612	4.718314007009	9.384863838182
Mo	13.604793051736	1.953822760415	9.394669711691
Mo	16.781510096108	1.951684718585	9.397971609536
Mo	15.191007903446	4.706113828911	9.398790466912
Mo	13.589268395983	7.454883359960	9.385846095705
Mo	11.999650571036	10.200068491742	9.362961891085
Mo	10.417707160593	12.948337609057	9.385151854452
Mo	7.258814042273	12.948542182095	9.382284518435
Mo	4.078181003238	12.956997037591	9.384795392303
Mo	0.895648408580	12.959976754215	9.386163670500
Mo	-2.287466281689	12.956469391271	9.386045012178
Mo	-0.699392457697	10.205666490971	9.385885564759
Mo	0.894723459338	7.456589775636	9.395120688627
Mo	2.485451123382	4.705804942500	9.398417251998
Mo	4.072263586852	1.953499853864	9.395517283558

81

H2SO4 initial

H	9.652480658411	10.007922360823	14.960443054478
H	8.311696614698	7.195201932670	15.212267847110
O	8.689051036708	8.498237304353	12.271078683856
O	7.377305631398	9.298755780561	14.308273330587
O	9.887859918519	9.486595831086	14.143615948724
O	8.764158085431	7.199599070046	14.323643265501
S	10.329139634034	5.726959547890	10.808782315632
S	7.183808839086	5.653635689872	7.683617099131
S	7.248314859319	5.726864226678	10.804736379468
S	11.974579848006	2.894717034281	7.748738380530
S	5.606208646993	2.892813831316	7.745627417489
S	7.246259381076	11.069562345421	10.798809676646
S	10.330087098603	11.067183886392	10.802657400607
S	11.869747582106	8.395732077286	10.808118368631
S	7.221754712784	11.158498526373	7.680408616219
S	5.619641114421	13.876573173146	10.861232220278
S	5.616947293187	13.906107893640	7.742931922443
S	8.788271227554	13.874687035695	10.863255737068
S	8.790020413448	13.909529334842	7.745440547004
S	10.359705950215	11.157730892104	7.683022450043
S	11.958556026099	13.878427944632	10.862268195925
S	11.961885493086	13.903528935779	7.744786621972
S	11.966885508247	8.370741646192	7.686821276398
S	13.519718221013	11.125122659644	10.835761935781
S	13.556824459753	11.146293253253	7.728872312202
S	13.535948694126	5.654546643143	10.869083525813
S	13.563191957645	5.638238613530	7.751979886759
S	15.124934761103	8.397928754557	10.864219373176
S	15.144040133358	8.385648728501	7.746505974554
S	15.140262491505	2.887741448119	10.882665639575
S	15.146020840839	2.894387774735	7.765133058521
S	16.735798979174	5.648523769858	10.880560056351
S	16.730811197593	5.639393900269	7.763476170284
S	18.327028771199	2.890040118232	10.879408183881
S	18.319127036743	2.892176665676	7.761985561640
S	11.954461562284	2.906767867435	10.865829132858
S	10.399250589275	5.654686411423	7.687220614704
S	8.791494255971	8.394660152823	7.623214512235
S	5.703870188996	8.394305423524	10.798765194498
S	5.614610718676	8.371999170306	7.679174966569
S	4.060589997480	11.124049190847	10.832040830646
S	4.021590921871	11.146831963979	7.724432397637
S	2.439630264339	13.897052925599	10.854381951840
S	2.436792129541	13.900542894409	7.742383993891
S	-0.744633675242	13.899355872678	7.742495054134
S	0.847895992076	11.141273736492	10.853829614013
S	0.845297772819	11.143395328942	7.740844674082
S	-0.745111078914	13.899111642914	10.854900315463

S	2.457820760137	8.397049456537	10.859057458946
S	2.430514423302	8.386393549898	7.741643927210
S	4.044511087747	5.656686916788	10.861111901433
S	4.017257593002	5.636560998682	7.743567724948
S	5.625929902862	2.908343380330	10.862101611625
S	8.789930724219	2.933270344933	10.837638923555
S	8.791811985646	2.890050947366	7.729993152774
S	8.539680991736	8.684417524649	13.690067000542
Mo	8.790429502409	4.762839970913	9.251339329580
Mo	7.202391904829	1.982594773557	9.297895172722
Mo	10.378625211746	1.982538382178	9.299907675546
Mo	11.958057956690	4.740767317348	9.296810049317
Mo	10.330202259591	7.505324734616	9.198751136480
Mo	8.790134043947	10.176220157235	9.194242643436
Mo	5.644111763430	10.211295672953	9.245302260133
Mo	2.442046164344	10.224344590396	9.294081554779
Mo	4.040383091501	7.477872714865	9.286201394579
Mo	7.248660487224	7.504827446974	9.194221412087
Mo	5.621946251675	4.740731265590	9.291661476588
Mo	13.554563813289	1.973653249148	9.315922118737
Mo	16.733035373786	1.971831096579	9.321300226874
Mo	15.141452829420	4.727561940428	9.324562596414
Mo	13.538306632791	7.477863584779	9.296458904915
Mo	11.934997925723	10.210665562856	9.250427363361
Mo	10.369647918788	12.967123001060	9.291158286514
Mo	7.208530704628	12.968279597759	9.288551823777
Mo	4.031401171672	12.976095909854	9.294149502936
Mo	0.846414018005	12.979922645859	9.298518861040
Mo	-2.338073844614	12.976626409280	9.297432644935
Mo	-0.748914610951	10.224456288100	9.297283445481
Mo	0.845896564890	7.478571475055	9.313853893119
Mo	2.439174041190	4.727668586763	9.318428930592
Mo	4.025093392187	1.973550092404	9.314039556769

81

H2SO4 transition

H	10.077275470410	10.115526665302	12.724673847007
H	8.274906198827	6.545830973695	12.952180822992
O	8.687693332436	8.524310909953	11.170673371783
O	7.327804711706	9.133924847827	13.455705415900
O	9.859266822547	9.345422675261	13.380511811631
O	8.935062851940	7.191845305863	13.376442130735
S	10.380044025977	5.686763249564	10.940453765645
S	7.184882339147	5.710993330399	7.888309558076
S	7.243466394287	5.668726273375	11.003537172870
S	11.971075014573	2.901908022115	7.827726648184
S	5.606798374489	2.928372573609	7.867080390188
S	7.185937816484	11.177917620525	10.984590967188
S	10.398563250904	11.147487881686	10.981902898064
S	11.938915395544	8.391220467249	10.941374402700
S	7.249809321949	11.136971046850	7.887563530752
S	5.601124613659	13.919158352875	10.965236345667
S	5.622346423215	13.906166759523	7.842281365808
S	8.778147461549	13.930844903026	10.987312345363
S	8.794650233968	13.916030222495	7.861216378532
S	10.319964437269	11.148164922997	7.896368168060
S	11.975394385890	13.916164096888	10.982350801232
S	11.950322052297	13.916190265589	7.862976125188
S	11.961243197269	8.401842735784	7.816527566390
S	13.555448222424	11.150126905086	10.954017502769
S	13.539585828886	11.162476879896	7.841148142536
S	13.554384295985	5.660332909879	10.945333489146
S	13.564338009831	5.654805460983	7.828064599230
S	15.136241323172	8.411001929171	10.951779195422
S	15.149095577801	8.409613761692	7.827642015104
S	15.134606401968	2.915468897987	10.962664731565
S	15.150779980465	2.902677164021	7.841951733714

S	16.722454058361	5.664765235941	10.962693256152
S	16.742083716856	5.656333811179	7.842290725809
S	18.315681714280	2.913188947204	10.980047872685
S	18.325183523559	2.908050011979	7.858898734669
S	11.963094805014	2.913652581783	10.951817870383
S	10.384785008671	5.666020793809	7.814982367648
S	8.777795468261	8.419975038805	7.888870998992
S	5.597826367772	8.409060220684	10.972302449259
S	5.653839776403	8.383663331148	7.879630030985
S	4.019273424941	11.162965263944	10.962394684840
S	4.043354079487	11.150955575160	7.844458953525
S	2.433986179352	13.914969535072	10.949563864325
S	2.436839435393	13.911451957197	7.833519091153
S	-0.752464217362	13.920754783106	7.845006839623
S	0.844471261834	11.161582353917	10.948839269857
S	0.848309863518	11.161980438476	7.832662407513
S	-0.738128628598	13.910740060368	10.959885777131
S	2.425577740325	8.417445043618	10.963750355347
S	2.443173364663	8.406565106710	7.838711809475
S	4.007797680394	5.666076807917	10.986842049238
S	4.030510066477	5.652480059270	7.863848572635
S	5.619408877488	2.905422900262	10.985394185751
S	8.800575778054	2.915075300778	10.954061446624
S	8.781415553936	2.920264399503	7.842600990493
S	8.539522511362	8.646935477696	12.832252357652
Mo	8.799133478413	4.760982769781	9.400891057476
Mo	7.200353017914	1.997048147875	9.409303342814
Mo	10.379708684877	1.992934001506	9.390636305252
Mo	11.971795404405	4.740645843675	9.381649053205
Mo	10.368149995861	7.492247508749	9.349089324108
Mo	8.785107724641	10.183091037342	9.476021475251
Mo	5.623104896933	10.238485633498	9.420552181814
Mo	2.438280343747	10.243942448710	9.395926156923
Mo	4.015382450665	7.486754657996	9.411167980352
Mo	7.254088838206	7.517219946220	9.457503642121
Mo	5.606311142820	4.752421107269	9.443417135541
Mo	13.553839207170	1.989320851908	9.397490659430
Mo	16.731482745964	1.994026917755	9.416194803718
Mo	15.146165946130	4.741742424952	9.394850881068
Mo	13.557535958096	7.490580428392	9.381749271754
Mo	11.958477448668	10.226501492878	9.400887988205
Mo	10.366800352999	13.012110008810	9.436851812762
Mo	7.205595370984	13.007657548439	9.416636352800
Mo	4.026293164831	12.993218494988	9.397351599856
Mo	0.845080202953	12.997198255517	9.392056905210
Mo	-2.336928016392	12.994950976163	9.407207623382
Mo	-0.744504596344	10.242783519223	9.390060050159
Mo	0.845920331484	7.496427470947	9.396935265989
Mo	2.434082105554	4.743478329492	9.416708998205
Mo	4.024252958425	1.994314436295	9.424348215807

81

H2SO4	final		
H	9.953821847922	10.071739530124	12.996037912753
H	8.004864296713	6.722636549408	13.247841907750
O	8.822164357104	8.419924420320	10.399398533289
O	7.352334972134	9.105753014150	14.582660712858
O	9.727468044002	9.468829291802	13.767139341566
O	8.787358072589	7.298543235671	13.483749749568
S	10.378601646137	5.726244388755	10.906035319522
S	7.212749769671	5.668011649544	7.800118292671
S	7.253687929353	5.724718335644	10.906873030125
S	11.993731697520	2.910960844510	7.830594618281
S	5.630800409289	2.913034240392	7.836805057592
S	7.264260188969	11.117425967484	10.904671669979
S	10.362577112717	11.107979941668	10.900597719657
S	11.922176517463	8.403984940323	10.907636923373

S	7.230810079012	11.173844056328	7.791238958229
S	5.645955812287	13.904315123793	10.947822946647
S	5.637168026816	13.921352596145	7.830288635607
S	8.808880933444	13.903222259533	10.950913076066
S	8.815577193413	13.928617189863	7.828502028859
S	10.393734900658	11.176782361467	7.796741402167
S	11.981207902934	13.904914687307	10.953189717376
S	11.986507966399	13.922317298222	7.836283776689
S	11.995013495682	8.401778167877	7.790592010086
S	13.555798203027	11.149825802351	10.937517811691
S	13.584964507410	11.168451675362	7.820025753500
S	13.563038349643	5.670309535920	10.948388828527
S	13.587610289917	5.658831596156	7.827281111420
S	15.150550978171	8.412108150129	10.950791973922
S	15.170532286302	8.409927956602	7.833761395689
S	15.163014533069	2.910581845532	10.961561961111
S	15.169948790735	2.912580968785	7.842625941174
S	16.754366271510	5.665644928677	10.963850352992
S	16.757907908967	5.661505449322	7.844710718643
S	18.345688447893	2.910479835921	10.965453704399
S	18.344437705883	2.913268399446	7.846111984620
S	11.983353050804	2.926843334085	10.948093882499
S	10.412542863722	5.665479821835	7.790688351218
S	8.812504589065	8.414350758635	7.645867157555
S	5.704904021986	8.408951755364	10.911520204627
S	5.635676915304	8.403132833047	7.797676756301
S	4.071356073565	11.153555976773	10.939067721935
S	4.043685134365	11.166675790856	7.820972143135
S	2.463517616181	13.919249281521	10.949096097104
S	2.458717159731	13.916702099637	7.834512083085
S	-0.720604654115	13.918074325825	7.837131163142
S	0.870645824865	11.160989133242	10.950710974588
S	0.871154489184	11.164032970657	7.836070828247
S	-0.722409392713	13.918831780671	10.950865064925
S	2.475977448495	8.413049572266	10.952423017652
S	2.459191353791	8.409655257722	7.835547776317
S	4.060518761296	5.672170936159	10.954484015669
S	4.040324337389	5.658748271228	7.832526883747
S	5.643386539724	2.925639744581	10.953594658660
S	8.815789709793	2.938040414294	10.937920997032
S	8.812261496762	2.906175843943	7.820822104643
S	8.209315188345	8.880595732292	13.414167070859
Mo	8.816949693714	4.762312298448	9.357320430002
Mo	7.224687560907	2.000778048140	9.391827452455
Mo	10.401672281958	1.999570529459	9.388744339429
Mo	11.985285975647	4.758671207024	9.377272312006
Mo	10.342670833429	7.532628706329	9.300296677283
Mo	8.810487264630	10.177391345568	9.299803536233
Mo	5.651169311477	10.241445131653	9.359137801123
Mo	2.465380502632	10.245558825477	9.391372350661
Mo	4.062712030560	7.494944554621	9.383746377187
Mo	7.289926562773	7.537145831610	9.307143257484
Mo	5.638451048109	4.758580382600	9.385473470671
Mo	13.578725797441	1.994456381053	9.396631371164
Mo	16.755829740625	1.993453233028	9.402853320362
Mo	15.165920496072	4.746949816621	9.401074926511
Mo	13.565245542294	7.494524473244	9.380195790812
Mo	11.979447202906	10.236546419302	9.354346220816
Mo	10.391595465611	12.994634461513	9.384603106383
Mo	7.233551410836	12.991824723064	9.376212697507
Mo	4.052923499528	12.996524697601	9.388761328166
Mo	0.870062873223	12.999728349450	9.394686745183
Mo	-2.313832934834	12.996358438792	9.391447137612
Mo	-0.723499526156	10.245385554789	9.390399671452
Mo	0.870734955336	7.497013689042	9.400487780689
Mo	2.460234169832	4.747322347189	9.405033133577
Mo	4.046911698161	1.994883460769	9.402858335829

TFSI+MoSe₂ initial

H	10.077351685056	6.669327682992	11.797467976228
C	9.241088497011	9.465475680246	13.354174502196
C	9.610902765807	5.592297120480	15.011472908744
N	9.361822096485	6.823999739253	12.542099636946
O	8.752354167362	8.611428457089	10.879267833513
O	7.076227993559	7.998153408541	12.730383308721
O	9.821619957607	4.380719043190	12.635161719525
O	7.512157957604	5.192316735777	13.375912901668
F	10.579498782569	9.488630282809	13.119715338708
F	8.705357965043	10.675996009601	13.049881265463
F	9.009061099914	9.182284429886	14.660141372733
F	10.879481224403	6.078040708453	14.962300291841
F	8.819616862001	6.449748346113	15.703193804167
F	9.613181556273	4.378446346044	15.619226174301
S	8.417137555733	8.191063488132	12.234846335964
S	8.940864971524	5.343617587728	13.263435207087
Mo	5.546436825082	4.767542425765	7.873459666601
Mo	3.894952866192	7.626694696785	7.868554972842
Mo	2.225847522243	10.496872515032	7.873118721283
Mo	0.557873533352	13.376658895138	7.874833282326
Mo	3.886056368267	13.372323913183	7.873931746234
Mo	7.205104191281	13.359568280998	7.872569253416
Mo	10.505748775124	13.358479802485	7.876339058374
Mo	3.878433938480	1.878051554997	7.892819273071
Mo	7.195743036304	1.887883730915	7.875050387283
Mo	8.852863664970	4.794204237719	7.836540493961
Mo	7.263535767579	7.666704253108	7.788806510420
Mo	5.575672327999	10.479091239347	7.831308508875
Mo	2.222581094578	4.754603841092	7.894529835642
Mo	0.558082123545	7.628636570011	7.889337116907
Mo	-1.110143899048	10.497431687853	7.875550073248
Mo	-2.769661746001	13.372611846167	7.877247431997
Mo	10.515425050080	1.889959295724	7.874548273581
Mo	12.173395807369	4.765570499536	7.868542533849
Mo	10.445881981377	7.676597837632	7.781483676620
Mo	8.856359554936	10.422964706935	7.789481139350
Mo	13.833455291907	1.877830591186	7.889969972443
Mo	15.492682782988	4.755608134583	7.894171334167
Mo	17.154413729003	1.874969809502	7.896161838381
Mo	13.812396019098	7.628525019442	7.872073600741
Mo	12.134297011399	10.480904467287	7.837270729026
Se	3.874035647610	5.705797584557	6.217594297647
Se	2.216721313812	8.577967733471	6.215620647747
Se	0.557009199910	11.456774453383	6.214294215544
Se	2.220485518113	14.336663395651	6.214587177667
Se	5.544808258374	14.337602881905	6.217579056144
Se	8.857415842856	14.338876425489	6.221371682116
Se	12.166406057047	14.337448970353	6.221334204056
Se	5.529139472828	2.839576584574	6.219057401672
Se	8.854603584845	2.842297728469	6.204598735604
Se	7.180145163328	5.731400735128	6.169885563359
Se	5.547865658963	8.559245856804	6.166267358552
Se	3.882521837999	11.457656671332	6.203215982747
Se	3.895742705360	5.722312987456	9.546683319160
Se	5.550087334432	2.853059083698	9.547024861754
Se	2.239539500379	8.587566588388	9.542368091411
Se	0.559340984480	11.455985009578	9.535120545736
Se	-1.105842472857	14.335501513599	6.215229707854
Se	-1.103798967192	14.336576825737	9.537055462926
Se	12.182982303950	2.838393401155	6.215567806395
Se	10.531581504314	5.731623338894	6.170261701136
Se	8.850297443137	8.588760945364	6.101025878081
Se	7.224388809982	11.463591475053	6.168417666871
Se	8.853826988889	2.876457618268	9.520053411563

Se	2.221477725831	14.336963622990	9.535225580058
Se	15.497361277453	2.837068431006	6.232366957097
Se	17.155391743151	5.708929289875	6.231114868797
Se	12.163556807693	2.852547383297	9.544776128523
Se	7.238612679168	5.795043889437	9.497100516738
Se	5.628192158070	8.581177088469	9.491802362223
Se	3.915803281345	11.437491773923	9.516386552285
Se	5.544915928208	14.314669682315	9.544411132390
Se	18.812094099124	2.836419441077	6.232918381698
Se	15.490470825415	2.834943395417	9.558728116043
Se	15.492026708060	8.578307955232	6.218810838735
Se	10.480668268242	5.800103315406	9.475400583545
Se	13.82736016761	11.458278845097	6.207207264523
Se	7.247236744749	11.375896711067	9.496925509319
Se	8.854329031321	14.313326844458	9.548770279936
Se	18.816952471429	2.835675654939	9.560590555812
Se	13.819388047407	5.721072294857	9.545828925668
Se	13.842728269703	5.709736324308	6.216879753770
Se	17.155381965363	5.715655026295	9.558263386585
Se	12.071344407145	8.583627577610	9.499481850449
Se	12.164259059678	8.565421486236	6.166617112836
Se	15.471927678154	8.587313552259	9.543476891664
Se	10.459861709484	11.374195413671	9.502423534642
Se	10.487879119158	11.464217356635	6.171189344398
Se	13.796580421675	11.438988539983	9.520066060336
Se	12.166197713594	14.315116563359	9.547614153058

90

TFSI+MoSe₂ transition

H	9.968116410231	6.571981958587	11.481520903852
C	9.502004955334	9.600952458226	12.705816664914
C	9.574548013268	6.025933625197	14.813540488224
N	9.274272789235	6.942267341680	12.183687904108
O	8.772776073233	8.459390726230	10.066073557572
O	7.159985181802	8.428332334352	12.179749433334
O	9.385006790966	4.483888348851	12.644544735407
O	7.293479952353	5.757271847091	13.387258564620
F	10.823047578254	9.538012471440	12.420234896587
F	9.022602545090	10.843134229749	12.474989843200
F	9.302540577012	9.272613014753	14.008127603612
F	10.869084584278	6.383015916116	14.596367938747
F	8.932718184771	7.015394412249	15.479402017962
F	9.536206852684	4.883234859356	15.547293618954
S	8.498959469086	8.338663587010	11.633290486119
S	8.714783749184	5.660594883951	13.163145000683
Mo	5.531800789022	4.668464132400	8.013189513483
Mo	3.863152105585	7.536283907067	7.995539693241
Mo	2.219759540102	10.414932577640	7.984989415555
Mo	0.558176045206	13.293864280351	7.979297638609
Mo	3.884563346964	13.291198394212	7.989168535505
Mo	7.199034665290	13.288019058067	8.012098539884
Mo	10.515787168533	13.291979651281	8.009738650833
Mo	3.878707314651	1.793081862695	7.997565272918
Mo	7.195620616829	1.799887415301	7.990624885685
Mo	8.849586734670	4.695178234831	8.003369874059
Mo	7.201380286195	7.548867196153	8.066685254287
Mo	5.559067047683	10.401128574788	8.006161060070
Mo	2.218624745377	4.665870497889	7.993728010946
Mo	0.556075316251	7.544091667496	7.984024456236
Mo	-1.104886577322	10.414578493087	7.984918936358
Mo	-2.765771624991	13.292140293734	7.991360829133
Mo	10.519965987619	1.802813066136	7.982340962124
Mo	12.201823592156	4.655143785925	7.979133726017
Mo	10.523023924513	7.558022089652	8.012681706760
Mo	8.863514167565	10.407221577965	8.045963996282
Mo	13.838477264022	1.788226235691	7.988052567776
Mo	15.501083957711	4.667140497965	7.986129190464

Mo	17.156490117928	1.791501248213	7.998561023614
Mo	13.833375930880	7.540407639773	7.991522117399
Mo	12.149904269057	10.397787870870	7.998893198876
Se	3.882049849896	5.620928596879	6.335387934502
Se	2.219797658165	8.498410533516	6.319349849784
Se	0.557729285974	11.373720305344	6.319267375286
Se	2.224371954338	14.251796861223	6.320815607327
Se	5.553156856214	14.238608654945	6.329842283879
Se	8.856501445412	14.240795206673	6.345000876250
Se	12.164944470662	14.247666172013	6.332813535850
Se	5.533841931475	2.763512092534	6.334387177711
Se	8.852105382290	2.778125149736	6.332818540950
Se	7.184231212768	5.677887280125	6.363888991527
Se	5.572695515384	8.469387799415	6.358920076348
Se	3.900755173538	11.364170722573	6.334665172832
Se	3.863927800934	5.624556820730	9.668485441011
Se	5.539003710348	2.744605547848	9.667269859298
Se	2.205943106375	8.504939619273	9.654927694033
Se	0.557744346546	11.378038729389	9.644043977914
Se	-1.107667497945	14.254590221789	6.323245028130
Se	-1.097545785263	14.249233498464	9.648893246663
Se	12.186111182525	2.746274823376	6.313065456823
Se	10.525387999370	5.658111043508	6.339097312222
Se	8.841955595536	8.501564145060	6.497438716419
Se	7.238160901230	11.357498717832	6.357293666650
Se	8.858804642784	2.756149500318	9.650259297020
Se	2.217062838977	14.253709884987	9.643716543056
Se	15.502799519508	2.745737893590	6.326010519686
Se	17.160177723049	5.623977532981	6.321853273513
Se	12.181706235181	2.745412796526	9.651781503097
Se	7.196642150810	5.616031776675	9.691287158969
Se	5.499476068631	8.502670676343	9.669651750608
Se	3.879320052831	11.372816320595	9.651897229781
Se	5.532688331246	14.250160881875	9.663642767413
Se	18.814082878781	2.747397419602	6.330965808231
Se	15.495063996474	2.753044630356	9.654891208913
Se	15.487541357949	8.498444533141	6.320757250115
Se	10.545331227864	5.617681674161	9.620623559316
Se	13.812845336440	11.367530096912	6.334001178559
Se	7.193757038139	11.359258782125	9.688926941445
Se	8.857270408759	14.254786606185	9.673366934945
Se	18.813470630300	2.752775264716	9.661731991961
Se	13.849133517221	5.620789719678	9.652448475844
Se	13.846593513770	5.628443600307	6.319806149798
Se	17.153630019219	5.628514313308	9.652200298893
Se	12.167604119603	8.500848911041	9.675691802187
Se	12.149558027615	8.479493842283	6.329605572170
Se	15.493089677738	8.502294811044	9.652105756900
Se	10.526939347903	11.363461633060	9.678014503593
Se	10.473497609257	11.362550251658	6.352235372235
Se	13.828765703335	11.369486925789	9.648359283961
Se	12.181293684571	14.249721524535	9.666271859025

90

TFSI+MoSe2 final

H	9.996233911790	6.959467841976	11.655600976036
C	9.743598381961	9.858800569334	13.552934578182
C	9.654512329967	6.134827355121	14.963246565171
N	9.464558585785	7.382704127614	12.445020225879
O	8.837077809533	8.445048211509	8.892769573111
O	7.500986079211	9.183766707299	12.198228620464
O	9.039102488320	4.929899792423	12.651622854245
O	7.342980262876	6.556131802630	13.658432255867
F	11.077652228872	9.579494337971	13.599879799377
F	9.579839972863	11.200605442080	13.355138541523
F	9.163391075461	9.509504010156	14.725909218640
F	10.979277175823	6.357408428818	14.746513855023

F	9.176172534882	7.066260961165	15.824379473936
F	9.484394062383	4.898104821900	15.502435299024
S	8.955429865799	8.993098806339	12.029915904320
S	8.692392933993	6.169992302701	13.321562325661
Mo	5.525721133373	4.629490802739	7.921993230494
Mo	3.879496270235	7.478932834132	7.914019101680
Mo	2.207117872071	10.354280401786	7.921701451655
Mo	0.538487887767	13.231839401074	7.927780496559
Mo	3.866015128304	13.225727481254	7.921277194867
Mo	7.192431167237	13.217145564462	7.910136413389
Mo	10.482692020925	13.219219022489	7.914297204982
Mo	3.859181396247	1.735016012459	7.934872861755
Mo	7.179107615158	1.743626668312	7.927941051076
Mo	8.831178876163	4.629062146674	7.898599139138
Mo	7.277283052125	7.542577698015	7.834918103223
Mo	5.536803889755	10.344732069629	7.888696837018
Mo	2.203711154665	4.610481127743	7.936930476421
Mo	0.539810335500	7.483005262406	7.934155910179
Mo	-1.130225406077	10.354468850712	7.925002263516
Mo	-2.787597327208	13.226468966810	7.924926517728
Mo	10.493659303112	1.745579206901	7.926488896273
Mo	12.155606221478	4.626470961964	7.920422379323
Mo	10.392650164910	7.547010684339	7.833954803593
Mo	8.835649414340	10.240991261396	7.834335791312
Mo	13.816206854850	1.733642484582	7.932351790873
Mo	15.473375419503	4.611069008403	7.938048349531
Mo	17.135883458547	1.731186343538	7.934266858222
Mo	13.793183356960	7.478298513950	7.921489445896
Mo	12.136095098571	10.348416434463	7.893745072932
Se	3.856165013155	5.561519390677	6.259543780375
Se	2.199981126254	8.435522725097	6.263061485398
Se	0.537214776683	11.313731058021	6.264966021919
Se	2.199136153644	14.192893919954	6.266136581958
Se	5.522613998782	14.191240440252	6.260774852190
Se	8.838968215973	14.197407183836	6.253933673674
Se	12.151953022264	14.192227419404	6.264068053525
Se	5.516198525039	2.698323501508	6.268494210127
Se	8.834830856864	2.693704051031	6.253558926890
Se	7.169069623767	5.578015094497	6.232170382275
Se	5.525124516710	8.426315640961	6.225642956522
Se	3.857947888558	11.314997513725	6.246869949623
Se	3.874776489298	5.578856416505	9.593381654690
Se	5.526351848989	2.710901519779	9.592408409175
Se	2.221933726028	8.440124399232	9.586757479114
Se	0.540312912363	11.309528415090	9.586210132198
Se	-1.122751116714	14.192203723398	6.267053869387
Se	-1.125069624630	14.191256964555	9.588844620548
Se	12.158825625915	2.697387646144	6.266221234075
Se	10.503281690535	5.577148157141	6.236097608909
Se	8.835131459368	8.441293834399	6.026962597434
Se	7.192870654523	11.314442140114	6.225019442109
Se	8.835083162109	2.723005273393	9.584022992317
Se	2.204703682594	14.191407860450	9.586359303521
Se	15.477009059972	2.694699929265	6.273147065497
Se	17.135783993999	5.565260226357	6.274491908539
Se	12.149926981765	2.707250996909	9.590341681522
Se	7.210066007968	5.652963366085	9.552887198632
Se	5.602019015482	8.430736142938	9.545710005561
Se	3.887261019341	11.298299480954	9.574218964282
Se	5.531936732433	14.170295977054	9.584545542208
Se	18.795280105322	2.693930740879	6.273090581263
Se	15.474102951469	2.688934385589	9.600022640810
Se	15.470211233134	8.434948086050	6.267711705045
Se	10.464790326960	5.645421230013	9.537578684586
Se	13.813939733370	11.315773575050	6.250771734229
Se	7.226233904497	11.250454823294	9.541116949373
Se	8.835548358597	14.171139879696	9.588434688148

Se	18.796586898288	2.690835283916	9.601241201338
Se	13.803363536674	5.574817610219	9.595815220067
Se	13.821251124145	5.564770696142	6.261428961785
Se	17.137200627711	5.569928279984	9.601937708056
Se	12.066203042649	8.434942394305	9.550341521049
Se	12.148531442851	8.428712742042	6.231551202925
Se	15.455444490531	8.439634624779	9.589635378384
Se	10.443103781013	11.251990177248	9.544093755040
Se	10.481118146729	11.316095926288	6.229063381495
Se	13.787217801842	11.300895004865	9.578366899201
Se	12.142835657080	14.173424004386	9.588447063744

76

O2 initial

O	8.695752621507	8.331593800015	12.759746159757
O	8.387455378663	9.035734603646	13.733983309149
S	10.326527789360	5.717482476360	10.861516762701
S	7.178110908887	5.658946143120	7.740226323542
S	7.241368505314	5.715960885366	10.861645688582
S	11.969402726479	2.895645421038	7.788672209771
S	5.599487405596	2.895432039698	7.788324118444
S	7.238362532237	11.070029777469	10.862843690407
S	10.331061654355	11.069199423365	10.863164656258
S	11.872094672617	8.395391614097	10.862998731730
S	7.219677971712	11.151251197575	7.741651544948
S	5.612899034638	13.881021454244	10.906902987139
S	5.615930012472	13.900286978187	7.789355681406
S	8.784878886957	13.879721860308	10.911142364074
S	8.784339043237	13.902464882327	7.793148482353
S	10.349700790613	11.151459215808	7.741416689510
S	11.956473687322	13.881076118121	10.906544254754
S	11.953395971510	13.900521243361	7.788931388028
S	11.955629454765	8.370913225934	7.740335177029
S	13.519254256378	11.128089634428	10.882192079095
S	13.548048329883	11.143657656606	7.775261960294
S	13.533782792266	5.651128879912	10.911128848160
S	13.554511951727	5.640224088988	7.793671242870
S	15.121426837987	8.397722234203	10.907984418846
S	15.137974985417	8.385194063568	7.790729072182
S	15.134833003964	2.888531733911	10.921065676093
S	15.141350706587	2.892588936099	7.803134749661
S	16.727489027241	5.646395914279	10.921715395402
S	16.727153029476	5.640397125708	7.803784966564
S	18.320238405463	2.888368873630	10.920843302778
S	18.313455291487	2.892292065679	7.802741953663
S	11.949722538051	2.902807707895	10.906145655461
S	10.390439566673	5.658891172490	7.739616213363
S	8.783753242596	8.394150431467	7.694149003883
S	5.694163602787	8.394974682567	10.863165640901
S	5.613392200787	8.370490667126	7.741350125988
S	4.050083743589	11.127859824817	10.882800482559
S	4.021856781624	11.143278040913	7.775429539942
S	2.432445862951	13.898177595035	10.896204094807
S	2.434302177399	13.897807258709	7.782906573550
S	-0.750611158526	13.898052903521	7.782724315691
S	0.841785596730	11.143464983786	10.897315572979
S	0.842063893647	11.140635131008	7.784093003602
S	-0.749240295395	13.898322970321	10.895964564051
S	2.447199755173	8.397284755472	10.907974978565
S	2.430874431060	8.384931316816	7.790680835947
S	4.034293060338	5.650244175544	10.910932999137
S	4.013761366734	5.639753037211	7.793280323447
S	5.618946637572	2.902585990638	10.905935986990
S	8.784488819441	2.925284734713	10.880344082258
S	8.784607407016	2.892466706652	7.773229164853
Mo	8.784235753364	4.760497710782	9.300997919598
Mo	7.195324702143	1.980911038665	9.338740186920

Mo	10.373792380479	1.980781206503	9.338882924154
Mo	11.952866345435	4.739278724485	9.341327964944
Mo	10.327277498506	7.502915905657	9.262100967492
Mo	8.784630070971	10.175376956270	9.264570147986
Mo	5.638993583304	10.210039750751	9.303386227962
Mo	2.437204259311	10.223907850346	9.341135692495
Mo	4.035212747981	7.476545756579	9.342122952440
Mo	7.241417202942	7.502663048868	9.263151290265
Mo	5.615408798394	4.738741451163	9.340892446779
Mo	13.549995157832	1.973296847028	9.355502547029
Mo	16.727556973163	1.970707462260	9.361640594789
Mo	15.135794743925	4.727034761573	9.362149302986
Mo	13.532917796547	7.477253985662	9.342315076378
Mo	11.930229626148	10.210079772235	9.303122603277
Mo	10.364773885885	12.965827534063	9.341498273788
Mo	7.204500948468	12.965849927233	9.341767709698
Mo	4.026424768315	12.976069937298	9.340218098543
Mo	0.841781418771	12.979685431302	9.338799739638
Mo	-2.343150749574	12.976419156625	9.339719721094
Mo	-0.753893825908	10.224152308397	9.340984944051
Mo	0.841229145717	7.477594544104	9.357163190794
Mo	2.432447144015	4.726774784446	9.361855299753
Mo	4.018821662653	1.973276407108	9.355138854404

76

O2 transition

O	8.753030612135	8.422754713343	10.619852872067
O	8.737825500441	8.425591129341	11.985256439234
S	10.336861391979	5.714889590490	10.998956521916
S	7.174067461604	5.654024024608	7.862999272392
S	7.198110492819	5.717367577498	10.987954854084
S	11.947857725544	2.915517911255	7.908941174982
S	5.597355242214	2.909008066992	7.901571908555
S	7.213766131425	11.127801431665	10.969467984195
S	10.318988794353	11.128230488178	10.978383069657
S	11.890879494870	8.411320631875	10.995669419841
S	7.185914429682	11.181685154030	7.844079674207
S	5.604163462245	13.901617988524	11.007968545909
S	5.591878557820	13.926824869748	7.889701846012
S	8.770600607827	13.906051950677	11.001305622194
S	8.775344183060	13.926682603628	7.883714952830
S	10.363677871092	11.177998514243	7.853650976965
S	11.938462284401	13.906917784567	11.013301754986
S	11.954643679366	13.920764450945	7.894837875662
S	11.959434504933	8.401312559348	7.870506756097
S	13.512065166812	11.154102842387	11.010113222810
S	13.539829957047	11.163193023902	7.896495022643
S	13.529434522441	5.667147100401	11.028706919456
S	13.535156027032	5.662111986636	7.911076424261
S	15.116866185296	8.413663638719	11.026777132745
S	15.121964734226	8.409949450269	7.908973772912
S	15.128094798668	2.905483982105	11.023269462986
S	15.123002716857	2.917786685655	7.904648244369
S	16.719238510978	5.663109861308	11.026794177495
S	16.710319656139	5.663525135031	7.907964384980
S	18.305026641394	2.910352641558	11.018651025328
S	18.306669394940	2.914653309616	7.899528095461
S	11.945841531605	2.914083790538	11.025883268148
S	10.374893625487	5.657310653025	7.874137761739
S	8.774100160876	8.410791311168	7.814279318363
S	5.644799781654	8.412627056841	10.975375610429
S	5.582252951961	8.401530429002	7.849334488465
S	4.032199860810	11.151760889177	10.994042387089
S	3.998854989172	11.167042315484	7.879464222280
S	2.424374491951	13.911235619822	11.017510603464
S	2.412697208277	13.920015531072	7.901096530254
S	-0.759183812450	13.916608588483	7.904013690982

S	0.832739345088	11.160040421390	11.019515531122
S	0.822073420268	11.163776575325	7.901816774017
S	-0.762511846496	13.915386327179	11.021251435725
S	2.432149615885	8.415522065068	11.013846400867
S	2.409679068725	8.409483532948	7.896696688118
S	4.016421705757	5.671245907211	11.011832868048
S	4.006106177957	5.658710474762	7.893748622174
S	5.598128214271	2.919268009154	11.018078456208
S	8.772011837241	2.934187726674	11.013439360774
S	8.773884572986	2.910349710530	7.899551242651
Mo	8.771639892580	4.765902316247	9.439226322326
Mo	7.184761721821	1.996446013913	9.462165067939
Mo	10.360442492268	1.996529774486	9.464308430280
Mo	11.940113174236	4.752599438986	9.466603738100
Mo	10.341937576363	7.506715910832	9.394958563167
Mo	8.768626228311	10.235460689467	9.374212477869
Mo	5.611161166380	10.239825629560	9.412901764070
Mo	2.420193000878	10.245773638620	9.451216040383
Mo	4.015083059261	7.500498150437	9.443886646821
Mo	7.193400077674	7.506002549203	9.380010164735
Mo	5.603202156343	4.751810122394	9.451509252496
Mo	13.537731120373	1.993963464709	9.462896984344
Mo	16.716036329574	1.995101357335	9.455644319685
Mo	15.124310897681	4.746805494059	9.470612617688
Mo	13.525187133367	7.499728913538	9.464658600475
Mo	11.929727874384	10.238694483626	9.432761677410
Mo	10.358275098563	12.991829075560	9.440316632287
Mo	7.186207185221	12.992996755728	9.434537536257
Mo	4.010235618801	12.997298072333	9.448084099843
Mo	0.828378113991	12.997624983089	9.462177761211
Mo	-2.352605282319	12.997258632416	9.458807983868
Mo	-0.765157640952	10.244951021762	9.464099534561
Mo	0.827201066819	7.496566273480	9.466602130447
Mo	2.419643569992	4.747411369370	9.460596754000
Mo	4.006689178860	1.993689904861	9.459697418247

76

O2 final

O	8.696366231738	8.504760993461	11.469674786484
O	8.174521617906	8.856327481365	12.572810227262
S	10.360441541586	5.695519589049	10.886340379737
S	7.182047430195	5.679853368302	7.800823990531
S	7.231641587211	5.690905673661	10.910852169693
S	11.969960395844	2.884982001471	7.802526535719
S	5.605169156319	2.900813078444	7.820828484045
S	7.207146947813	11.125542097131	10.917332843688
S	10.352808242054	11.105226291973	10.914312778975
S	11.910209618064	8.379024028210	10.887621873187
S	7.222542914908	11.146857912239	7.803501865735
S	5.603122187071	13.897445328329	10.933456049675
S	5.612030868883	13.897219965547	7.813333700414
S	8.784000987779	13.893838719384	10.941192665054
S	8.786473770851	13.899205684272	7.821664834441
S	10.337412471115	11.141840183550	7.806679185220
S	11.961735353785	13.888628753419	10.938408629537
S	11.954647033955	13.898739143343	7.821417568006
S	11.981150589859	8.386333750982	7.756981918601
S	13.529969448485	11.129838608529	10.916875286435
S	13.542528736462	11.146068722541	7.808195543133
S	13.544254692825	5.647023097215	10.917995105395
S	13.565475438491	5.637057044026	7.801632917741
S	15.128166068689	8.394236700326	10.926444051408
S	15.150915903923	8.392154011900	7.805814447135
S	15.136611546107	2.893161825790	10.936923092397
S	15.147685274770	2.888682055460	7.817474777442
S	16.727127232534	5.645583275957	10.939173013713
S	16.738115483813	5.640943462395	7.819854435591

S	18.320563593288	2.891081212004	10.944805654661
S	18.321027567166	2.892532824179	7.826157950640
S	11.956968041089	2.902742223864	10.923428293391
S	10.394173217178	5.634480053529	7.752642845174
S	8.783460901504	8.400772108376	7.777215689423
S	5.642732912781	8.400024295065	10.917458643678
S	5.621783519757	8.375548692689	7.801828409633
S	4.033517692655	11.140091461198	10.923461651487
S	4.022880994687	11.144683561044	7.808760046963
S	2.429679584121	13.903528544168	10.925030128953
S	2.429481451117	13.897601384547	7.809200961294
S	-0.751194412534	13.900269762726	7.813651946008
S	0.837962705367	11.145252055555	10.926606017773
S	0.841813233293	11.146134020582	7.810919896013
S	-0.747736818964	13.899910300262	10.929577792890
S	2.433292471736	8.400689027826	10.936295167336
S	2.435929418773	8.392010257919	7.816356848201
S	4.027696591903	5.648902607259	10.942425804024
S	4.021747108744	5.644707561710	7.823720378722
S	5.619395794307	2.900055456577	10.937948907602
S	8.790471551259	2.921419399100	10.912887133659
S	8.781500014658	2.898565750904	7.804416883240
Mo	8.792055796351	4.758371850881	9.340945097509
Mo	7.197841147393	1.981704619002	9.370925467920
Mo	10.374962197531	1.981062723250	9.362704243671
Mo	11.964078037135	4.727284005185	9.351126332930
Mo	10.385615857601	7.468963844973	9.272820892409
Mo	8.762420976170	10.192482571686	9.363959886019
Mo	5.626348103953	10.221688874461	9.355997443934
Mo	2.433573498869	10.228844712208	9.371072302880
Mo	4.024744889950	7.480994492365	9.379309171135
Mo	7.223253586202	7.516584094351	9.354552725794
Mo	5.615612489342	4.738917521266	9.379700295590
Mo	13.552012761354	1.974598745130	9.372087600855
Mo	16.730749485174	1.973316487596	9.383408109706
Mo	15.143835281943	4.725352377767	9.373493433300
Mo	13.551726772274	7.476820030219	9.353152652170
Mo	11.938991641792	10.210496579506	9.347300380169
Mo	10.367436986868	12.973364623597	9.379808523858
Mo	7.196214263210	12.980381358874	9.377132516635
Mo	4.021061338138	12.980498898863	9.369234309982
Mo	0.840206406522	12.982021342941	9.369187295183
Mo	-2.340339134188	12.978047916250	9.372303602704
Mo	-0.751142901220	10.225656667270	9.365728050818
Mo	0.845020393963	7.478364197150	9.375750278289
Mo	2.436015489548	4.727681195571	9.385419893171
Mo	4.021895162697	1.975562023296	9.383806074688

90

TFSI	initial		
H	10.299129628553	7.231681353992	14.579932680679
C	8.132439876194	5.560297542800	16.717909019340
C	8.247095228451	9.516459517111	15.190167770318
N	9.290194458057	7.028932213382	14.677318372015
O	8.039760513837	4.817050216745	14.133145211320
O	10.312879565831	4.842092421548	15.300879102839
O	6.940627607871	7.572222626363	13.847977496512
O	8.980850553992	8.681494227833	12.767773698881
F	8.909014446802	6.270790656885	17.577251446070
F	6.936170115114	6.180280345217	16.571116432891
F	7.946136489955	4.305663370453	17.200543133533
F	7.625528916789	9.109516086177	16.323621593245
F	9.525353238701	9.887623077035	15.480581259881
F	7.580874645803	10.568331152351	14.653832113901
S	8.997393905224	5.392467022879	15.045377438050
S	10.298313265258	5.743255882100	10.973415050993
S	7.156430188885	5.677952735065	7.839242050737

S	7.216285052929	5.747340996070	10.958046248230
S	11.944482729776	2.919635004677	7.901503932084
S	5.577281793710	2.916708099673	7.895483682265
S	7.212303585925	11.090030319320	10.960748781467
S	8.268041001729	8.133332273690	13.902318581033
S	10.302329249820	11.094573233224	10.963407981887
S	11.847198026729	8.417124886085	10.968672536849
S	7.196891449439	11.178952993753	7.838897180614
S	5.589060719962	13.900675558380	11.013246479152
S	5.589601693441	13.927556390158	7.896128450276
S	8.760252518753	13.899814983915	11.016230412874
S	8.761052897258	13.928283717458	7.898350927653
S	10.327502130618	11.175631445433	7.843948913928
S	11.931273814723	13.903736423403	11.013981689354
S	11.931849504855	13.924915912104	7.896093398662
S	11.930782557434	8.392217569054	7.849121115370
S	13.493235535877	11.149679991326	10.990105405479
S	13.522944987767	11.166622159037	7.882904691806
S	13.509999794846	5.674821961548	11.022349304801
S	13.529235145452	5.660717681434	7.904808600056
S	15.098593290584	8.419651380205	11.014918977314
S	15.112471708850	8.407127907235	7.897783455494
S	15.112480949573	2.910715792603	11.031468058226
S	15.116433832985	2.915810194182	7.913768182079
S	16.706665007677	5.670117741657	11.028677977667
S	16.701788441477	5.661210767386	7.911358446295
S	18.297930095475	2.912686145994	11.028469708343
S	18.290368758590	2.914314174958	7.910820414144
S	11.924496848867	2.925546057870	11.019041148229
S	10.367610684503	5.680907447466	7.850462514228
S	8.763043063610	8.417157250550	7.790236313401
S	5.670712718990	8.421742132239	10.951099499354
S	5.586931744154	8.394132764377	7.833265092179
S	4.028596855345	11.147502597421	10.982767335766
S	3.993095813132	11.170472106289	7.875521334513
S	2.408396893765	13.919798694868	11.005174780671
S	2.407593435446	13.923839365596	7.891887778661
S	-0.775083716611	13.921875806758	7.892566765127
S	0.818817577040	11.164032811264	11.003061093836
S	0.814329430254	11.165158554247	7.890567606623
S	-0.773948664749	13.921476369764	11.005285244995
S	2.427019860296	8.419632194438	11.009346538560
S	2.402858656063	8.408068943399	7.891392544034
S	4.013917593825	5.677740062839	11.013153959707
S	3.989758514300	5.659812593445	7.895025519936
S	5.595753441908	2.930277474886	11.014123401489
S	8.758886603981	2.951286393831	10.991932703959
S	8.761026343680	2.915402776784	7.883317822709
Mo	8.759979655558	4.784399366465	9.409518832673
Mo	7.171635810563	2.005109284970	9.449176330962
Mo	10.348363532796	2.004883845054	9.450747045524
Mo	11.928078951568	4.762354076239	9.454604777100
Mo	10.298594142902	7.527274915377	9.367864412904
Mo	8.759217954930	10.197976467117	9.361445758328
Mo	5.614522949839	10.235196254625	9.396637308352
Mo	2.412344141673	10.246530100122	9.443516209505
Mo	4.011146681611	7.500209896046	9.438797253151
Mo	7.216365277522	7.526786803907	9.354535479113
Mo	5.592891023470	4.763131828011	9.443747059894
Mo	13.525367755721	1.996743255016	9.466919204020
Mo	16.704232241672	1.993822723332	9.470398116114
Mo	15.112074775821	4.749612082646	9.473002287173
Mo	13.509066254182	7.498945117016	9.450613510678
Mo	11.904804078186	10.233208885537	9.410352010774
Mo	10.341140604899	12.989861816628	9.445467415933
Mo	7.179979976593	12.989585589647	9.444599054175
Mo	4.001000253794	12.999665414264	9.445816119119

Mo	0.816825602658	13.002692887658	9.447715817755
Mo	-2.367513417404	12.999147722913	9.448847918139
Mo	-0.779123007983	10.246427923621	9.448550282001
Mo	0.817365469322	7.500107152351	9.462685733142
Mo	2.409993926705	4.749967327096	9.467896252069
Mo	3.996439095883	1.996835426818	9.463625735928

90

TFSI	transition		
H	10.407436598734	7.024221620643	13.347287474691
C	9.069531345120	5.960486742554	16.407214180023
C	9.021159982750	9.578109728774	14.294553722937
N	9.497426387742	6.976184812152	13.847398016376
O	7.990010197713	4.888398208100	14.202623693963
O	10.534899411951	4.799898933978	14.478635989804
O	7.054133305957	7.744611817684	13.831112610208
O	8.528690804851	8.244724743028	11.732246184973
F	10.122963529904	6.726286050674	16.789599060806
F	7.912289505511	6.638769556872	16.597494615694
F	9.051866013531	4.811223519075	17.129240886903
F	8.827065406212	9.301630808622	15.607100090473
F	10.346268398825	9.733488733034	14.053988898095
F	8.341094004156	10.689434051265	13.952927654360
S	9.252978467205	5.460923421130	14.596123241906
S	10.032252284677	5.422896370189	11.177837339013
S	6.851488112227	5.471659557847	8.068674759570
S	6.883431611653	5.454750636439	11.194796045349
S	11.640456029155	2.689586073307	8.072428079431
S	5.273435292223	2.693986617471	8.077489883522
S	6.849232452471	10.933252816012	11.210350060248
S	8.349341989523	8.070879991673	13.274983843909
S	10.043936113652	10.947609745744	11.204711004557
S	11.622306408918	8.186935085146	11.221822688601
S	6.908781226856	10.937599492069	8.090611627794
S	5.272126954832	13.695469536855	11.202553244403
S	5.287864603811	13.694680053353	8.079167686023
S	8.455289360410	13.702249199474	11.210605361200
S	8.456170110681	13.699628146500	8.090609318238
S	10.007655015001	10.933828010114	8.099680984909
S	11.637650872267	13.699696409102	11.207473286001
S	11.628514628651	13.696158602352	8.082708528108
S	11.610914231102	8.166252296823	8.099624452800
S	13.213981036663	10.941730643496	11.201617171707
S	13.202021491364	10.931514129024	8.093239732149
S	13.222880888511	5.431110323465	11.210356633871
S	13.230930113283	5.443103532222	8.089400733584
S	14.814374370399	8.194258170505	11.212120856045
S	14.806083025321	8.186509613730	8.089391325298
S	14.809124177680	2.687314311794	11.206655167556
S	14.815154609269	2.691928075416	8.086700398747
S	16.403058150479	5.441511621589	11.209530173530
S	16.400754810594	5.441484631095	8.089070249694
S	17.991921179632	2.691220161139	11.207133647968
S	17.987844855009	2.691855519113	8.087009596691
S	11.628862833599	2.683712460716	11.198525546207
S	10.060119903910	5.474951139639	8.077709489212
S	8.461498410549	8.200079611420	8.225304034587
S	5.295696896483	8.199155200704	11.196590845759
S	5.296475559123	8.169097502789	8.073574517293
S	3.698708623871	10.939339024342	11.186615261870
S	3.700526676854	10.936582061609	8.077496357040
S	2.101029267608	13.697988506863	11.187514151099
S	2.102494768093	13.694631747540	8.071910641579
S	-1.083424108132	13.693208989035	8.076370151725
S	0.515173755791	10.946476934344	11.194193659601
S	0.506760615506	10.937444593041	8.078659250210
S	-1.073463893084	13.698438537731	11.192076194348

S	2.106204040356	8.197665094676	11.204485226756
S	2.100594030878	8.186971423319	8.080619226094
S	3.693669028547	5.442654801908	11.205062252357
S	3.687775905746	5.441081017805	8.086811625368
S	5.285467462072	2.690972413670	11.201733857081
S	8.454961283547	2.701155923050	11.182189946409
S	8.452762583838	2.699180157764	8.071061874449
Mo	8.450518521181	4.545393699951	9.621627755364
Mo	6.865070111119	1.775985530320	9.632213357014
Mo	10.045036325583	1.776458288459	9.628547048258
Mo	11.642232579469	4.517360360194	9.637304083666
Mo	10.038749965996	7.267840242382	9.664076790457
Mo	8.448695526577	10.025109622509	9.678280471252
Mo	5.298729991977	10.014509191044	9.631230076696
Mo	2.103276348354	10.023886536085	9.635648273684
Mo	3.690492899398	7.275512552193	9.642471905855
Mo	6.864484832250	7.273460547401	9.643553673036
Mo	5.278775090699	4.525930631317	9.641211097319
Mo	13.222014532367	1.770963134438	9.640117251019
Mo	16.400745608615	1.774810949858	9.648578778773
Mo	14.813826715892	4.523515976839	9.650064857273
Mo	13.225000594680	7.268650976223	9.656289976854
Mo	11.609097820730	10.012765891663	9.655035199031
Mo	10.042920607978	12.787443740823	9.648630303838
Mo	6.869133071501	12.782561573014	9.649384793034
Mo	3.693799863102	12.777665796768	9.632697715716
Mo	0.511411392811	12.778131926701	9.630872525141
Mo	-2.670089224327	12.776992737049	9.642167364392
Mo	-1.081017098353	10.022816589462	9.645170255956
Mo	0.514286709408	7.276641771344	9.648125828053
Mo	2.103424621676	4.525251953227	9.647990285865
Mo	3.692597208922	1.773789515599	9.643521736067

90

TFSI	final		
H	10.873791529595	7.054533947269	13.749040588394
C	9.226925971857	5.807396661367	16.555356755068
C	9.370859782687	9.652389070584	14.802369030542
N	9.954384663545	7.091995389470	14.225733272280
O	8.224981176066	5.154712563076	14.179564831616
O	10.705905501587	4.736341531898	14.581134288439
O	7.498952680650	7.998571448331	13.740810459181
O	8.556597944501	8.279385309342	10.663873017319
F	10.318435504513	6.377457833443	17.130827332145
F	8.139232786139	6.592513383209	16.760892970423
F	9.010601911284	4.582931695463	17.109383944052
F	9.037741381432	9.295851307653	16.063899858800
F	10.714332431214	9.897952703571	14.735659629512
F	8.692980996471	10.785951136655	14.459975132212
S	9.510154294082	5.549085909110	14.709938080172
S	10.123693969328	5.596742405436	11.134000465848
S	6.966785701282	5.549103374831	8.022348567705
S	7.003297196912	5.605110947302	11.139021691533
S	11.753526902808	2.794661494410	8.068913517943
S	5.386249403516	2.792780042915	8.066326013020
S	7.015348029007	10.987568915934	11.156320964796
S	8.912902908732	8.327708073267	13.479188616641
S	10.118108787689	10.992630158032	11.158456999547
S	11.678102778121	8.283535017561	11.154467280641
S	6.995940686778	11.053190452648	8.042492912315
S	5.400138889509	13.787961104983	11.190849434821
S	5.401211114621	13.800916581800	8.074953230279
S	8.569620096396	13.786698849637	11.195905107292
S	8.570949464193	13.803944423164	8.074724549203
S	10.146370678442	11.051075166784	8.047579593481
S	11.739533476855	13.791105727775	11.192505872879
S	11.739967452657	13.79375486998	8.075763574630

S	11.744889248065	8.287460705226	8.043121579743
S	13.315151802971	11.037920461395	11.181843014389
S	13.333777130109	11.049769576985	8.064596812357
S	13.319716690916	5.550375453045	11.190331639985
S	13.342790080174	5.543871270184	8.067712864614
S	14.909986136605	8.295655694360	11.189222083004
S	14.921003630468	8.294162790800	8.073433706235
S	14.922025490907	2.793979544441	11.200542015418
S	14.927045126775	2.794402247196	8.082237680180
S	16.515465523804	5.549512418184	11.197247751710
S	16.511057269723	5.545424437046	8.078639071458
S	18.105933330341	2.796417129553	11.198386833334
S	18.099141124120	2.792832349653	8.079648097131
S	11.737990690353	2.809111472310	11.187193557764
S	10.168402555334	5.551310486918	8.030577434293
S	8.567702304989	8.298292681195	7.885439140869
S	5.455527278386	8.284975165533	11.143052161459
S	5.389075866838	8.288046689821	8.027314887380
S	3.826335151465	11.034447544998	11.174328486409
S	3.802011520808	11.052150095774	8.057282470022
S	2.218193650072	13.805265655646	11.184397796014
S	2.218124972798	13.801121176553	8.070625628163
S	-0.966598916205	13.799260646736	8.071212957394
S	0.628244153098	11.046907318803	11.185400166306
S	0.623716389489	11.047782960896	8.071495621351
S	-0.963709677305	13.805981729870	11.18558449546
S	2.233446277886	8.296573401962	11.184050581473
S	2.211780240421	8.295437999072	8.066870833277
S	3.819724722842	5.555195267883	11.181845991437
S	3.795068608567	5.542271886012	8.060125476370
S	5.401011316144	2.812014234511	11.183997490094
S	8.567377635266	2.822928352008	11.171565987184
S	8.568627653913	2.787039512363	8.051307071007
Mo	8.563088892348	4.642718885592	9.586207769426
Mo	6.980857872529	1.883770334223	9.623026836537
Mo	10.157459857671	1.885186861623	9.623708216966
Mo	11.742698163399	4.640273598449	9.616692988323
Mo	10.089708156584	7.412725006765	9.546511424135
Mo	8.567034498800	10.052707550610	9.557011852480
Mo	5.406319804540	10.120695556510	9.595301401331
Mo	2.220524632966	10.129911630996	9.624629672259
Mo	3.816848071217	7.378708199465	9.612619948147
Mo	7.035648531501	7.410393609888	9.538119737141
Mo	5.396454261859	4.641894533320	9.611251997279
Mo	13.336264955823	1.877229547661	9.637230728634
Mo	16.513668720138	1.874927578203	9.641608338341
Mo	14.922648625480	4.630343093237	9.639649947214
Mo	13.320820617625	7.375746260306	9.623783506927
Mo	11.731166436857	10.122836633617	9.607621240465
Mo	10.148353113734	12.871139110685	9.629287498012
Mo	6.992043156983	12.869854083286	9.627935768251
Mo	3.810207409960	12.880198977501	9.627327855635
Mo	0.626125561056	12.884557459166	9.628541884155
Mo	-2.557198694506	12.880247859834	9.631019781428
Mo	-0.969243940543	10.129622499090	9.629867316728
Mo	0.626190526618	7.381196340178	9.634681581680
Mo	2.216986764032	4.630528612354	9.634823891599
Mo	3.803550976884	1.877327280159	9.635725790079

89

MoSe2+TFSIminus initial

C	8.635602277801	9.427707391338	13.511937854448
C	9.468059724597	5.597564882859	15.016074835494
N	9.331208319681	6.926704837333	12.641273868310
O	8.703454524919	8.687224833316	11.006586795347
O	6.861607342430	7.757516084883	12.465095762166
O	10.027539541491	4.548411400657	12.655426627180

O	7.611880706978	5.036062343285	13.189331567828
F	9.966233901068	9.739075289102	13.547939701563
F	7.940495212298	10.550675734953	13.132707872420
F	8.232433454249	9.088012064570	14.772480059939
F	10.679381529774	6.213575362762	15.182480549261
F	8.524910475920	6.311683165628	15.702197380056
F	9.544340171962	4.348184929070	15.575354821922
S	8.276044098923	8.062290000133	12.267994286583
S	9.009631675148	5.449773597502	13.190655457706
Mo	5.525732102247	4.796026821803	7.967090132631
Mo	3.875001739989	7.654576782551	7.961707136312
Mo	2.203052578337	10.522949617242	7.972309785322
Mo	0.535298017334	13.402609678080	7.978000352614
Mo	3.861597868779	13.397254505821	7.973995031540
Mo	7.181598751839	13.381967197889	7.968173725659
Mo	10.481301146278	13.380190323195	7.974214774692
Mo	3.857071029518	1.903634670754	7.993202391932
Mo	7.175235895145	1.917148793806	7.977026744099
Mo	8.834094104514	4.827168853757	7.928088732022
Mo	7.245985376094	7.696654147415	7.867150337984
Mo	5.552668607474	10.504047606076	7.918813979144
Mo	2.199974853495	4.782605847059	7.994162997989
Mo	0.533881284338	7.655984790656	7.991158540505
Mo	-1.134224784029	10.523076543177	7.978808162012
Mo	-2.792106367922	13.396932704960	7.979998466996
Mo	10.489643350030	1.917634969233	7.979063633332
Mo	12.135347746508	4.799213985618	7.970937342459
Mo	10.411794110838	7.697925627616	7.869180446747
Mo	8.830191569507	10.433575929164	7.870971085181
Mo	13.806439695912	1.905273435947	7.992716361958
Mo	15.464492110750	4.783196364300	7.997460845190
Mo	17.129659391600	1.899868207069	7.997134637118
Mo	13.784728713935	7.656018163445	7.974699192431
Mo	12.108610537627	10.503480135491	7.934425816953
Se	3.849807393475	5.731588545545	6.314165582018
Se	2.190751416728	8.604428096491	6.315374407339
Se	0.531945947387	11.483417064383	6.317553034853
Se	2.195848402885	14.364922341886	6.318348884687
Se	5.518997851659	14.365784297021	6.319405833782
Se	8.834408529294	14.364828665559	6.321164232149
Se	12.145024083947	14.361538225741	6.323870387868
Se	5.508152098131	2.863806921952	6.319296232925
Se	8.833470904708	2.867782289714	6.305199634913
Se	7.157765780978	5.754800351446	6.258677319341
Se	5.522715406741	8.585469079245	6.252917729697
Se	3.854961718270	11.486088447315	6.299249615299
Se	3.879489913909	5.752613447171	9.643636509168
Se	5.530204881064	2.885903818816	9.646374692619
Se	2.222540321050	8.612891176571	9.640233472698
Se	0.537748347735	11.480855395659	9.636576781794
Se	-1.127782240505	14.362143034315	6.319918692491
Se	-1.125868391154	14.365459607762	9.639159506168
Se	12.155242501136	2.867901450868	6.321575111193
Se	10.507465959927	5.757737014498	6.259041028960
Se	8.829779259229	8.609557068495	6.156593090971
Se	7.201339222341	11.489730490573	6.258654417819
Se	8.831777793804	2.917550711134	9.624090671741
Se	2.199037261507	14.363582494775	9.638021351471
Se	15.470506787311	2.864465273509	6.337145402357
Se	17.128125643078	5.735569176586	6.335135359432
Se	12.133911568810	2.886703974355	9.649165114899
Se	7.221918547252	5.834085185682	9.585537139610
Se	5.619569047215	8.606918022999	9.579060381821
Se	3.899245186665	11.458504925413	9.612634047582
Se	5.522592299024	14.336969355067	9.643529657483
Se	18.788627715845	2.862141615018	6.335962186815
Se	15.464442243243	2.861168944890	9.660554618685

Se	15.466095326024	8.604437946647	6.322874106020
Se	10.437952580594	5.843017518648	9.588976662369
Se	13.805056767854	11.483296222308	6.309810743457
Se	7.229085023072	11.387754746846	9.586733126308
Se	8.829611361796	14.333146972117	9.647355386192
Se	18.794655298313	2.862406768194	9.659708432061
Se	13.784153380784	5.749405914739	9.649742988369
Se	13.812922798272	5.736635711461	6.322286080004
Se	17.131328411386	5.742237275173	9.659128892888
Se	12.028827667532	8.603445478752	9.596716242559
Se	12.140470495896	8.589049743475	6.264885144312
Se	15.445005826214	8.612597459917	9.646459577120
Se	10.424873007063	11.385346964646	9.595576839441
Se	10.466039108452	11.487590148823	6.266693620805
Se	13.767525468881	11.460569788433	9.621711438180
Se	12.140857867463	14.338165845523	9.647486433288

89

MoSe₂+TFSI minus transition

C	9.295529340746	9.499348418690	12.603243517705
C	9.388555029721	5.961100807152	14.777277767937
N	9.369340840776	6.895294857227	12.181445437582
O	8.642983518514	8.364197351576	10.009876536818
O	7.057695192493	8.145448775488	12.164056577290
O	9.925197394513	4.513440883326	12.646921247022
O	7.533585056781	5.260485737878	13.014668020612
F	10.620679695383	9.587096565954	12.337892239394
F	8.683051575094	10.675684755096	12.309756779271
F	9.132199248951	9.247114186816	13.934657625904
F	10.652020130026	6.468459913109	14.878194727044
F	8.508139804128	6.856934268081	15.310529377477
F	9.322406056636	4.805148102594	15.509414566044
S	8.431086986382	8.055681687067	11.679566061001
S	8.958464936753	5.545762174267	12.990195584764
Mo	5.423143551935	4.723468072854	8.118687100239
Mo	3.768727642389	7.584369595241	8.111272050417
Mo	2.121578357949	10.472751458834	8.082295265530
Mo	0.458268744746	13.347415673966	8.070396253612
Mo	3.781635077941	13.344525855622	8.072789246625
Mo	7.096914403682	13.345770385180	8.075590753938
Mo	10.415629958546	13.348050529826	8.074869492557
Mo	3.783659383799	1.848847454187	8.083780247087
Mo	7.101958173161	1.858547999831	8.086020411361
Mo	8.765549320956	4.737854276875	8.113489899817
Mo	7.174840293647	7.651483274504	8.239714061847
Mo	5.447808549109	10.469756706641	8.095898613011
Mo	2.121988871712	4.724707901174	8.090367489856
Mo	0.456243949234	7.601099504831	8.082217229981
Mo	-1.206254167914	10.470808541954	8.076737369880
Mo	-2.864321082604	13.346497952261	8.074309685321
Mo	10.415675807496	1.856786165130	8.074182431366
Mo	12.096682988105	4.712347658795	8.064393044970
Mo	10.375023829397	7.651374334441	8.136663021043
Mo	8.774693475330	10.445021636634	8.082324000629
Mo	13.731310981753	1.844080470084	8.067856450037
Mo	15.396128682081	4.724549939594	8.073626830900
Mo	17.055247525447	1.847864753584	8.075045936435
Mo	13.727726438909	7.589389237011	8.089034228944
Mo	12.055627151509	10.460949941179	8.078892824942
Se	3.789000907154	5.684102500147	6.437847804739
Se	2.133922989843	8.549604375744	6.427153175481
Se	0.459654838761	11.424877688243	6.414062411457
Se	2.119407169732	14.307689658955	6.410269119187
Se	5.442009315366	14.297096572411	6.406428439903
Se	8.755345228053	14.301451466130	6.414392176513
Se	12.073483744944	14.309645427732	6.412054094587
Se	5.444289556746	2.829842379433	6.430565601808

Se	8.753037807557	2.841230386174	6.426412227892
Se	7.099239914719	5.768587663911	6.516937515573
Se	5.510037770746	8.509115652991	6.504705117258
Se	3.794031894920	11.414821424511	6.420047653857
Se	3.763634778879	5.675411356465	9.779574428445
Se	5.439521602737	2.792123377446	9.764174217195
Se	2.104462111318	8.563576701606	9.756767818585
Se	0.454867357523	11.443400673526	9.737779424592
Se	-1.203058889697	14.314847426120	6.415052675874
Se	-1.199572405874	14.302452716583	9.737187718379
Se	12.073477158248	2.804597505446	6.398792494624
Se	10.412140685350	5.737168015773	6.455649734259
Se	8.737435165966	8.545038098887	6.521278863210
Se	7.121771622766	11.411677000158	6.427082419188
Se	8.766072980777	2.804658836591	9.758386819649
Se	2.119451916461	14.306960217011	9.731913142744
Se	15.397413065694	2.806514070359	6.409519553928
Se	17.062803526037	5.683473942536	6.418508859693
Se	12.078928915174	2.803175536276	9.739247807420
Se	7.097806568599	5.651467364109	9.792832411553
Se	5.399644653667	8.584665408692	9.782844240571
Se	3.779148407289	11.437014299029	9.747099376226
Se	5.437429102308	14.302777715631	9.739479921113
Se	18.719933958201	2.811474265971	6.420160306970
Se	15.391495039874	2.804021456660	9.733972201633
Se	15.383143463394	8.549778514030	6.419076413309
Se	10.457231720163	5.684939088669	9.725762073257
Se	13.719978477695	11.421080696688	6.415944028484
Se	7.114579960041	11.408091540868	9.744900886020
Se	8.755155500557	14.303257020646	9.739983368170
Se	18.710088104094	2.801153315625	9.745948288402
Se	13.738523371724	5.671038737296	9.744984257881
Se	13.740581752978	5.687367279344	6.408204308416
Se	17.047547323930	5.680446904182	9.744929926232
Se	12.061757145433	8.568716782590	9.772528321703
Se	12.027489176832	8.522649987476	6.443924269870
Se	15.385940880016	8.558115673232	9.745962500332
Se	10.412708908968	11.410859718900	9.741943576180
Se	10.387887907699	11.421716767450	6.415112620854
Se	13.724060881578	11.426728063848	9.735106223865
Se	12.074100851037	14.297841664876	9.743793508325

89

MoSe ₂ +TFSI minus final			
C	9.157432149885	9.514306204768	13.085926818504
C	9.331659058950	5.836186426236	14.831946519132
N	9.089570524804	6.948218750956	12.285021047923
O	8.795185370212	8.549367506658	8.993993416834
O	6.818291074704	8.155803444826	13.019434728981
O	9.870156249347	4.620177731364	12.563680913625
O	7.458416685215	5.115513295609	13.102625314201
F	10.452421621509	9.511533795669	12.634443740980
F	8.626115089816	10.764671869756	12.820871114217
F	9.170671803023	9.342826250651	14.437266053883
F	10.593540185293	6.369012962175	14.927533928689
F	8.465358370979	6.677251772209	15.469643872467
F	9.327073589012	4.635224958091	15.501225948200
S	8.039385593853	8.216261965058	12.165033828304
S	8.847093910702	5.565113812632	13.025269018847
Mo	5.479041885316	4.744698788889	8.044809010222
Mo	3.831968743330	7.593578473190	8.043988376946
Mo	2.158662561919	10.468374829043	8.055750247356
Mo	0.490396117195	13.346260456552	8.060861342626
Mo	3.815689275502	13.338626217071	8.054876122303
Mo	7.142334143326	13.326093772522	8.046028620236
Mo	10.432845679245	13.329427395234	8.045286917560
Mo	3.812596540059	1.850108662192	8.064055438569

Mo	7.133398502439	1.861657969094	8.056554746910
Mo	8.794319534521	4.749615633662	8.021959378192
Mo	7.233703068134	7.655398546069	7.953383414636
Mo	5.488618888115	10.456439131551	8.018425933555
Mo	2.155579535344	4.726997775698	8.065204949911
Mo	0.490459935535	7.598961538602	8.063008400155
Mo	-1.178629165444	10.469183230706	8.054764858532
Mo	-2.835353537412	13.340167095403	8.056042709045
Mo	10.443824243424	1.860094420197	8.055405951578
Mo	12.098317169472	4.743542136575	8.032456274861
Mo	10.347351889852	7.652238179253	7.944987174999
Mo	8.788632686497	10.347620691506	7.955251040083
Mo	13.763438669785	1.848637026316	8.059794560757
Mo	15.421944660404	4.726710937655	8.061718387838
Mo	17.085177916131	1.844859398008	8.064952304146
Mo	13.7436647554695	7.594105696907	8.041055578137
Mo	12.086920310976	10.457967471536	8.016025176214
Se	3.807215641751	5.678515416535	6.387482403864
Se	2.152421872666	8.551828723779	6.395568183253
Se	0.490487952334	11.428896068760	6.398497889953
Se	2.150013537805	14.305378578710	6.398678720395
Se	5.473574755354	14.301023854699	6.395419835180
Se	8.786731508443	14.308432243257	6.389134729070
Se	12.102847474706	14.304878269051	6.396900388627
Se	5.469333919588	2.811580500396	6.396089441144
Se	8.788559250926	2.808827971039	6.381179874692
Se	7.124173179151	5.691609567248	6.355162093267
Se	5.476555804888	8.539853042693	6.353999850927
Se	3.808136516923	11.428755243117	6.380391896453
Se	3.831894971287	5.692580893710	9.722273253447
Se	5.482270412225	2.831221458673	9.721184111416
Se	2.173994273811	8.552101731007	9.718311774253
Se	0.489752667758	11.423443818755	9.718696242462
Se	-1.169716251251	14.307085328306	6.400060592671
Se	-1.173275794603	14.310317534646	9.719616544945
Se	12.106548918960	2.806188853460	6.389531772886
Se	10.453768980542	5.690030815493	6.343666234383
Se	8.786045788867	8.554196826298	6.139244564482
Se	7.143201284126	11.427139859178	6.356348752156
Se	8.790633678787	2.848019508258	9.714405917821
Se	2.155178206548	14.309579080125	9.718766695174
Se	15.426685402056	2.806947177857	6.402337569160
Se	17.087424534939	5.681630926126	6.403014092852
Se	12.095296772171	2.833718257341	9.715966890152
Se	7.167510951147	5.767765843787	9.673081485912
Se	5.564329695564	8.540480537157	9.672962709839
Se	3.841227706021	11.410203032647	9.707065689733
Se	5.480848453608	14.286914795513	9.716572131294
Se	18.745919604793	2.807780469062	6.404899427577
Se	15.419833144896	2.806862918185	9.726580403604
Se	15.424555653064	8.552725413958	6.394305065110
Se	10.420872652498	5.772558979192	9.666475188811
Se	13.767600893392	11.431626289843	6.379854482736
Se	7.183831726167	11.346850891397	9.674534328008
Se	8.786810105842	14.282981557663	9.720693692114
Se	18.748794937656	2.806727662183	9.729555014986
Se	13.742277692318	5.690251131619	9.714880101395
Se	13.773415420745	5.679989165410	6.381175174535
Se	17.084434174286	5.684299064380	9.728535859261
Se	12.009076981124	8.537835955233	9.670018840444
Se	12.101924287935	8.542911047588	6.348640796781
Se	15.400466610796	8.551976607173	9.716143843401
Se	10.392398097840	11.352663836869	9.669766893539
Se	10.431111160890	11.430146009056	6.355462155479
Se	13.733416958875	11.410081523799	9.706182198775
Se	12.093769030199	14.287101714456	9.718304148951

TFSIminus initial

C	9.722018794404	5.570855135187	16.163852936576
C	9.119234776543	9.381219384661	14.364154240413
N	9.523282815826	6.817524993493	13.748186991428
O	7.886607417092	4.897902633151	14.368803367825
O	10.325138961467	4.471603385413	13.850494732101
O	7.070393306367	7.741644001313	13.852169836289
O	8.642135386426	8.353895305000	11.974978252353
F	10.967086368275	6.120373514301	16.308318331725
F	8.818850621082	6.373513269218	16.802550284369
F	9.716641826506	4.345724093875	16.781617237064
F	9.037259495072	9.134884894720	15.705412495899
F	10.421584579724	9.640238602474	14.047145093706
F	8.372918957892	10.494676115119	14.082935303466
S	9.271768586771	5.349069420058	14.351682459667
S	10.243052498009	5.725845235610	10.897605460391
S	7.078998765674	5.687997374445	7.803049265487
S	7.131390417903	5.714175579999	10.918508930144
S	11.867309874853	2.911017878027	7.832690024880
S	5.502497251455	2.912826546896	7.839364053831
S	7.131244058138	11.099036378732	10.917918876239
S	8.441102326621	7.921640495877	13.388731331588
S	10.234756367915	11.096334411361	10.919323129409
S	11.784737355243	8.412624835597	10.921629192233
S	7.119576358460	11.168419721162	7.796399891318
S	5.511552759618	13.903020532655	10.955441638442
S	5.512839785611	13.919614419138	7.836616293411
S	8.683283175096	13.899383291246	10.959080924695
S	8.685880592512	13.923148607588	7.842896461390
S	10.249404071339	11.169036826752	7.798401445162
S	11.857502701309	13.900725552941	10.959006040644
S	11.857461234981	13.919635593907	7.840919252437
S	11.853741197977	8.391522542108	7.796632129593
S	13.421797027121	11.148176720262	10.936981157799
S	13.447624193640	11.163116373483	7.829797664111
S	13.431574546700	5.667888042420	10.957739405013
S	13.458661200432	5.660831212345	7.838757427914
S	15.021885558855	8.415962458578	10.958734815843
S	15.039656897734	8.407540345806	7.840958884215
S	15.032818530879	2.908513615790	10.968118112673
S	15.042099245063	2.911958714691	7.851712058043
S	16.626596293614	5.665696807444	10.970693874460
S	16.629246720465	5.661165962909	7.853886140710
S	18.220585839130	2.907794494460	10.970863699459
S	18.216373645480	2.911401664728	7.854424322217
S	11.850720296174	2.924714300923	10.954740980735
S	10.288421138029	5.682950595539	7.788926067850
S	8.680442426816	8.411916286052	7.785658694417
S	5.575059864386	8.417006518042	10.922938086358
S	5.521380200923	8.385305143563	7.803973314277
S	3.947944721055	11.149745891777	10.935003354172
S	3.921898352132	11.162127190945	7.826715203641
S	2.333739809481	13.921081762077	10.947821402793
S	2.332104870710	13.918296954056	7.834699903211
S	-0.848660868432	13.917827089020	7.836522829541
S	0.742838781065	11.163432919812	10.949893751788
S	0.741687611657	11.162049499358	7.836976002430
S	-0.846739491358	13.920173265169	10.949696744402
S	2.346044738646	8.417372142407	10.959260295570
S	2.331056696035	8.406432101479	7.840963162208
S	3.934600008288	5.669043840894	10.962559790869
S	3.913624142575	5.658372386023	7.843719858010
S	5.521234515582	2.920737271835	10.959404614209
S	8.687267732201	2.946622785118	10.935984803738
S	8.684515982936	2.914820908213	7.824123157574
Mo	8.685792285721	4.779095570505	9.354769417941

Mo	7.098488511835	2.001519812183	9.391102607790
Mo	10.273433267205	2.002416630234	9.389573916208
Mo	11.856285199333	4.754030372810	9.381756850890
Mo	10.236422057296	7.520626335311	9.323869741777
Mo	8.683926940045	10.202245849212	9.324693451469
Mo	5.535861997733	10.229961411797	9.358851816050
Mo	2.336759732623	10.244649046128	9.392621597391
Mo	3.931528540499	7.495182812399	9.393617089935
Mo	7.136734307258	7.522978707574	9.341265915808
Mo	5.512433972964	4.753281030989	9.391923196832
Mo	13.447630098569	1.992867256933	9.401645108971
Mo	16.627930902155	1.990911339160	9.410670619595
Mo	15.036424607178	4.747096953039	9.409567033004
Mo	13.436608937302	7.496244363446	9.391186858381
Mo	11.832018148478	10.230212847136	9.360585460610
Mo	10.267054772130	12.987880261892	9.391568939976
Mo	7.101556442748	12.988561602813	9.388784767393
Mo	3.924940080172	12.996511201596	9.390085467470
Mo	0.742597263911	13.000045216087	9.392258003415
Mo	-2.440633611675	12.996246865837	9.393562152151
Mo	-0.852814688098	10.244577634212	9.393784115845
Mo	0.741656420570	7.498534315467	9.407232003956
Mo	2.333218816023	4.746513767257	9.412349115661
Mo	3.921988216268	1.991885148388	9.406941122242

89

TFSIminus transition

C	9.617830976542	5.744136889290	16.022913060587
C	9.163082372943	9.354891673895	13.894699908750
N	9.494379771724	6.780792976420	13.498019365045
O	7.868977973414	4.890431470367	14.202856557925
O	10.339840745233	4.455874941211	13.844535506511
O	7.047012693671	7.755632937521	13.473282642536
O	8.605607429497	8.180728836966	11.314913799044
F	10.818776303889	6.381236825461	16.151831097029
F	8.642886909122	6.525790900140	16.571613075099
F	9.672154079517	4.566333456975	16.718695298168
F	9.014545941600	9.114614470152	15.231042683972
F	10.475399282495	9.540277363878	13.627081503944
F	8.457681296680	10.466307266007	13.573736078095
S	9.249824768895	5.342273367481	14.219152086335
S	10.317009049881	5.641574091436	10.969981656304
S	7.107502738140	5.730216933876	7.961470459803
S	7.118475709741	5.609968750559	11.042590887714
S	11.875261928854	2.903767679329	7.856303524430
S	5.525882579824	2.922543230064	7.890803608367
S	7.125538406401	11.143528485075	10.981865783202
S	8.426649948339	7.816530531336	13.007098497624
S	10.274473407386	11.137832009968	10.987674251478
S	11.860108515509	8.427332635615	11.029574346631
S	7.123182569984	11.146583649754	7.867554164209
S	5.522689306175	13.908694247821	10.982990206575
S	5.523488752881	13.906505351928	7.858633427532
S	8.695571416589	13.907424536370	10.984775365302
S	8.701412057791	13.912890648463	7.869739168426
S	10.268812708264	11.154633030565	7.864414938776
S	11.873998447705	13.901035436492	10.994617829202
S	11.876784556481	13.915325339605	7.871639902876
S	11.827181484509	8.372081210214	7.910849201826
S	13.454332382330	11.157193413111	10.989701255466
S	13.453199831661	11.147796855864	7.877430455135
S	13.463569819371	5.642398977410	11.000334880541
S	13.471026436763	5.664796063480	7.876291196660
S	15.045447136799	8.410715292752	11.005522400346
S	15.042280206550	8.398741469447	7.888421687832
S	15.049603210022	2.897548447412	10.986226773251
S	15.059100618120	2.908684227973	7.869097255138

S	16.635317681706	5.652998303663	11.005121059215
S	16.651695975702	5.659292605713	7.887008840041
S	18.227490039291	2.894484149252	11.000855459422
S	18.239018460384	2.912244781345	7.883095854824
S	11.880533962885	2.895366464434	10.984951651284
S	10.282797336334	5.709459185274	7.907289468661
S	8.676755490664	8.388070542455	7.983302838660
S	5.497669639111	8.445934734380	11.040786454304
S	5.586485538891	8.358445893455	7.955843072303
S	3.936668424166	11.167676552224	10.993727591848
S	3.942775539527	11.141706333207	7.876936803936
S	2.347953777663	13.911467650993	10.980164427447
S	2.343672624202	13.909354010068	7.864988123208
S	-0.835423680855	13.915145325388	7.873045454426
S	0.753022349686	11.164178007731	10.992348186470
S	0.755509649378	11.149609502506	7.876577144272
S	-0.830864357180	13.906033006940	10.988321962742
S	2.334498875740	8.416177221469	11.014847341968
S	2.361483813287	8.396400695168	7.897231618113
S	3.924794584439	5.647131034720	11.033859535626
S	3.943207473793	5.660554137239	7.908156355089
S	5.525343509001	2.884113908503	11.014223918403
S	8.709995917348	2.894916383411	11.000577341693
S	8.694478828651	2.926074811040	7.878042464295
Mo	8.704436259304	4.743600037056	9.455773928198
Mo	7.114470679145	1.990130083138	9.438653355237
Mo	10.288825970179	1.989748213952	9.424004594283
Mo	11.891325030881	4.728690497084	9.421030335428
Mo	10.251587938452	7.529123096750	9.500722477519
Mo	8.709251574588	10.234387373858	9.414995553089
Mo	5.532110896311	10.239109302821	9.444134974584
Mo	2.346889828052	10.241343832705	9.441071538092
Mo	3.933718322179	7.480546944450	9.477046158924
Mo	7.163722924832	7.522067891633	9.586718507566
Mo	5.513170568524	4.734842207780	9.474225050182
Mo	13.463348334273	1.983170309066	9.418976173570
Mo	16.643833913764	1.987347177329	9.430127427103
Mo	15.054748010998	4.739290903877	9.435622698776
Mo	13.454923664505	7.482506045771	9.454476932590
Mo	11.856877478714	10.234036037965	9.436344750201
Mo	10.286857571304	12.993700584515	9.426228762720
Mo	7.109914969851	12.994157554851	9.419466901780
Mo	3.936333136886	12.991399588871	9.422870307594
Mo	0.755663846801	12.992360452947	9.425914402808
Mo	-2.425006004655	12.991388020535	9.430416665355
Mo	-0.838512497384	10.239787544662	9.437642140947
Mo	0.753934189073	7.491771109527	9.448012414613
Mo	2.347612866052	4.739189108952	9.453936875223
Mo	3.937630055915	1.984828459894	9.441069920940

89

TFSIminus final

C	9.606625783762	5.561316489925	16.190330691369
C	9.127625449098	9.327908049115	14.286484601562
N	9.389978717790	6.791337964864	13.751857738801
O	7.969949479689	4.705603042481	14.290854341680
O	10.464974040121	4.558987290443	13.918458384700
O	6.955380139387	7.729977773260	14.399814236981
O	8.724214823274	8.423449991488	10.440124249690
F	10.840585173214	6.122935554664	16.411417234848
F	8.661771987421	6.367660133142	16.759571974422
F	9.576810925679	4.348216984898	16.838630848403
F	9.217425851702	9.201318850866	15.640025809365
F	10.391054343976	9.462521967340	13.774513530660
F	8.438993645627	10.490594642201	14.007270258864
S	9.292283913903	5.330991738234	14.344553158215
S	10.279451712728	5.735283075895	10.938583511295

S	7.115210379576	5.674939755377	7.838077656551
S	7.161312805075	5.737921306979	10.958168821740
S	11.884986196951	2.914317789920	7.865918760028
S	5.535299328725	2.923383134390	7.877252704100
S	7.163759097440	11.111290700836	10.944111335897
S	8.143419638218	7.852084072300	13.507947419804
S	10.262663573083	11.116030027210	10.937062507052
S	11.818173236697	8.409148657081	10.940833920410
S	7.130526650089	11.172951622218	7.827387103565
S	5.542879946159	13.9065558385919	10.982208102294
S	5.532721720493	13.920471450262	7.867257891186
S	8.709657623575	13.901131474858	10.980279710770
S	8.708389307715	13.928546617688	7.860863568039
S	10.289292336928	11.177062990804	7.822843093583
S	11.876233416295	13.905130228336	10.983049956894
S	11.887818962084	13.927224669081	7.868288646072
S	11.890111429629	8.405861724238	7.820810289628
S	13.448882917406	11.152185399346	10.969347077180
S	13.482595410243	11.172917448152	7.853087787439
S	13.454085714320	5.674862912254	10.981337322232
S	13.481000413342	5.661913384462	7.859329229905
S	15.043354422039	8.413473655171	10.982413193544
S	15.067489915070	8.412294765427	7.867503325831
S	15.057957038299	2.912851062009	10.992496130805
S	15.063953291825	2.915170432407	7.876376905386
S	16.650651821996	5.668035387432	10.996907227529
S	16.657281630043	5.664365275832	7.880196830256
S	18.244174230057	2.911961392965	10.997387698254
S	18.244930769124	2.918117504365	7.881228944485
S	11.878694639205	2.935859517070	10.985751300139
S	10.305717477671	5.670105579196	7.821297404909
S	8.710724977513	8.418421639334	7.682641378204
S	5.612804126672	8.413298765099	10.954450939734
S	5.537758367329	8.403314175956	7.834618344862
S	3.970567374269	11.153610253253	10.974080443075
S	3.940484301567	11.168664916557	7.857988974016
S	2.359785904974	13.924058765358	10.987672019886
S	2.354117375780	13.922514350646	7.874462031307
S	-0.820343785545	13.925785753217	7.875332187629
S	0.765510877845	11.161778077737	10.985968161315
S	0.768820895309	11.167543254669	7.872950868394
S	-0.825822457540	13.923153601070	10.988374732174
S	2.375352573641	8.414846259116	10.988407414656
S	2.361636626919	8.411131219095	7.873697341193
S	3.964249747110	5.677114919774	10.994223291623
S	3.946488916848	5.664218147329	7.873583420845
S	5.544497782633	2.933193018187	10.993305956200
S	8.714165769417	2.948873806892	10.983178656709
S	8.709746022302	2.914610880460	7.861798414458
Mo	8.715809183648	4.771886513820	9.398260407941
Mo	7.125554202723	2.008008091300	9.432282601012
Mo	10.296713391761	2.006683245384	9.429129613663
Mo	11.877680399925	4.763770760700	9.408657550128
Mo	10.242142602891	7.534916137282	9.331478454382
Mo	8.713641437465	10.182344170786	9.336330398074
Mo	5.550584248422	10.241072946144	9.393220678842
Mo	2.362744982896	10.247484459825	9.427762822636
Mo	3.966412787773	7.499581070250	9.423325365713
Mo	7.190610614262	7.539647332635	9.345700834664
Mo	5.545973721604	4.768059073064	9.427191231015
Mo	13.471855986608	1.997498469455	9.429624466780
Mo	16.652738360773	1.995247746543	9.433637041483
Mo	15.060790936525	4.750796728915	9.433273177362
Mo	13.459193572969	7.498158068823	9.410773451733
Mo	11.872584075815	10.242379282858	9.384402687024
Mo	10.290034517740	12.992701858069	9.409991710559
Mo	7.130151455132	12.989696528230	9.412430230704

Mo	3.948518639292	12.998617117692	9.425762442567
Mo	0.766824132730	13.003164453463	9.432485347929
Mo	-2.414773813128	13.000380555513	9.424712508954
Mo	-0.827676565926	10.247822680452	9.423607373008
Mo	0.768559344069	7.499939659404	9.434637949793
Mo	2.361290287287	4.751851705797	9.440459747755
Mo	3.948103885803	1.999905612822	9.436284010430

References

- 1 P. Jurečka, J. Šponer, J. Černý and P. Hobza, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1985–1993.
- 2 F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2012, **2**, 73–78.
- 3 A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098–3100.
- 4 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.
- 5 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
- 6 F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057–1065.
- 7 S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787–1799.
- 8 I. Frank, J. Hutter, D. Marx and M. Parrinello, *J. Chem. Phys.*, 1998, **108**, 4060–4069.
- 9 H. Nan, Z. Wang, W. Wang, Z. Liang, Y. Lu, Q. Chen, D. He, P. Tan, F. Miao, X. Wang, J. Wang and Z. Ni, *ACS Nano*, 2014, **8**, 5738–5745.
- 10 P. K. Gogoi, Z. Hu, Q. Wang, A. Carvalho, D. Schmidt, X. Yin, Y.-H. Chang, L.-J. Li, C. H. Sow, A. H. C. Neto, M. B. H. Breese, A. Rusydi and A. T. S. Wee, *Phys. Rev. Lett.*, 2017, **119**, 077402.
- 11 Y. Liu, P. Stradins and S.-H. Wei, *Angew. Chem. Int. Ed.*, 2016, **55**, 965–968.
- 12 J. C. Slater and J. C. Phillips, *Phys. Today*, 2008, **27**, 49.
- 13 S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200–1211.
- 14 J. Klimeš, D. R. Bowler and A. Michaelides, *J. Phys. Condens. Matter*, 2010, **22**, 022201.
- 15 G. Henkelman, B. P. Uberuaga and H. Jónsson, *J. Chem. Phys.*, 2000, **113**, 9901–9904.
- 16 G. Henkelman and H. Jónsson, *J. Chem. Phys.*, 2000, **113**, 9978–9985.
- 17 J. J. Mortensen, L. B. Hansen and K. W. Jacobsen, *Phys. Rev. B*, 2005, **71**, 035109.
- 18 J. Enkovaara, C. Rostgaard, J. J. Mortensen, J. Chen, M. Dułak, L. Ferrighi, J. Gavnholt, C. Glinsvad, V. Haikola, H. A. Hansen, H. H. Kristoffersen, M. Kuisma, A. H. Larsen, L. Lehtovaara, M. Ljungberg, O. Lopez-Acevedo, P. G. Moses, J. Ojanen, T. Olsen, V. Petzold, N. A. Romero, J. Stausholm-Møller, M. Strange, G. A. Tritsaris, M. Vanin, M. Walter, B. Hammer, H. Häkkinen, G. K. H. Madsen, R. M. Nieminen, J. K. Nørskov, M. Puska, T. T. Rantala, J. Schiøtz, K. S. Thygesen and K. W. Jacobsen, *J. Phys. Condens. Matter*, 2010, **22**, 253202.
- 19 A. H. Larsen, J. J. Mortensen, J. Blomqvist, I. E. Castelli, R. Christensen, Marcin Dułak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. B. Jensen, J. Kermode, J. R. Kitchin, E. L. Kolsbjerg, J. Kubal, Kristen Kaasbjerg, S. Lysgaard, J. B. Maronsson, T. Maxson, T. Olsen, L. Pastewka, Andrew Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. S. Thygesen, Tejs Vegge, L. Vilhelmsen, M. Walter, Z. Zeng and K. W. Jacobsen, *J. Phys. Condens. Matter*, 2017, **29**, 273002.
- 20 A. H. Larsen, M. Vanin, J. J. Mortensen, K. S. Thygesen and K. W. Jacobsen, *Phys. Rev. B*, 2009, **80**, 195112.