

Supplementary Information

Nanostructured Pt-Doped 2D MoSe₂: An Efficient Bifunctional Electrocatalyst for both Hydrogen Evolution and Oxygen Reduction Reactions

Shrish Nath Upadhyay¹ and Srimanta Pakhira^{1, 2, 3*}

¹ Department of Metallurgical Engineering and Materials Science (MEMS), Indian Institute of Technology Indore (IIT Indore), Khandwa Road, Simrol, Indore-453552, MP, India.

² Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore-453552, MP, India.

³ Centre for Advanced Electronics (CAE), Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore-453552, MP, India.

*Corresponding author: spakhira@iiti.ac.in (or) spakhirafsu@gmail.com

Periodic Calculations:

1. 2D Monolayer Pristine MoSe₂:

_chemical_name_common	'BG_MoSe2'
_cell_length_a	3.234700
_cell_length_b	3.234700
_cell_length_c	20.000000
_cell_angle_alpha	90.000000
_cell_angle_beta	90.000000
_cell_angle_gamma	120.000000
_cell_volume	181.229393
_space_group_name_H-M_alt	'P -6 m 2'

_space_group_IT_number

187

loop_

_space_group_symop_operation_xyz

'x, y, z'
'-y, x-y, z'
'-x+y, -x, z'
'x, y, -z'
'-y, x-y, -z'
'-x+y, -x, -z'
'-y, -x, z'
'-x+y, y, z'
'x, x-y, z'
'-y, -x, -z'
'-x+y, y, -z'
'x, x-y, -z'

loop_

_atom_site_label

_atom_site_occupancy

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_U_iso_or_equiv

_atom_site_type_symbol

MO001	1.0	0.000000	0.000000	0.000000
SE002	1.0	-0.333333	0.333333	-0.082650

2. Pt-MoSe₂ 2D Monolayer:

_chemical_name_common

'BG_Pt_MoSe2.out'

_cell_length_a

6.738619

_cell_length_b

6.739656

_cell_length_c

20.000000

_cell_angle_alpha

90.000000

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_cell_angle_beta          90.000000
_cell_angle_gamma        120.000000
_cell_volume              786.627723
_space_group_name_H-M_alt 'P 1'
_space_group_IT_number    1

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loop_
_space_group_symop_operation_xyz
  'x, y, z'

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loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
MO001      1.0      0.008906      -0.008846      0.083631
SE002      1.0      0.344751       0.168236      0.002489
SE003      1.0      0.344755       0.168173      0.164785
MO004      1.0      0.004106       0.493562      0.083636
SE005      1.0      0.318097      -0.318049     -0.003679
SE006      1.0      0.318175      -0.318120      0.170922
MO007      1.0     -0.493493     -0.004101      0.083636
SE008      1.0     -0.156610       0.156763      0.002685
SE009      1.0     -0.156601       0.156750      0.164582
SE010      1.0     -0.168829     -0.345020      0.002547
SE011      1.0     -0.168726     -0.344985      0.164738
PT012      1.0      0.472110     -0.471004      0.083596

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Finite Non-periodic Molecular Cluster Model Systems with their Equilibrium Structures

1. Hydrogen Evolution Reaction (HER) on MoSe₂:

(i) [MoSe₂]

Mo	-0.18984100	0.00445200	-0.13167900
Se	-0.25439600	-0.27754200	2.29221800
Mo	2.12028100	0.00108000	1.37411900
Se	2.92413500	0.08026200	3.82022100
Mo	5.37956700	0.03187600	3.06236700
Se	6.01045700	-0.10728100	5.54609800
Mo	7.94729200	0.05773000	4.07836500
Se	-0.37372500	-0.34069300	-2.51365800
Se	1.37078100	1.87719900	-0.18660900
Se	1.36948600	-1.88561500	-0.16371400
Mo	2.10974500	0.02996900	-1.75832100
Se	4.11457300	1.66919900	1.50224000
Se	4.16221200	-1.56985000	1.45425500
Mo	5.03888200	0.09213600	-0.27437800
Se	7.05290800	1.91535600	2.75062600
Se	7.08535900	-1.83142300	2.76995100
Mo	7.99907900	0.04577200	1.31807300
Se	2.41764700	0.64322100	-4.20182900
Se	3.98983600	1.78948400	-1.83523600
Se	4.00822300	-1.62222200	-1.83401700
Mo	4.79889300	0.04318300	-3.54860100
Se	7.02209800	1.68406500	-0.43850900
Se	6.98342200	-1.55400600	-0.42882800
Mo	7.68291900	0.02995900	-2.33755700
Se	10.04928200	-0.08670100	2.85641900
Se	5.04947700	-0.31158700	-6.13264900
Se	6.51921300	1.90462900	-3.61960100
Se	6.56915500	-1.85958300	-3.63046100
Mo	7.17779600	0.04300400	-5.04990000
Se	9.63484300	0.11383200	-0.65788100
Se	9.44411300	-0.22054500	-4.18249600

(ii) [MoSe₂]⁻

Mo	-0.26783400	-0.00992700	0.01730500
Se	-0.27286400	-0.01384600	2.44960500
Mo	2.09841300	-0.00279300	1.42860300
Se	2.94712900	-0.00318600	3.84007900
Mo	5.38276400	0.00813800	3.04631600
Se	6.00806400	0.00565300	5.54756600
Mo	7.94214700	0.01689400	4.07252900

Se	-0.58290200	-0.00769100	-2.39501600
Se	1.30390200	1.88048200	-0.08076600
Se	1.31889800	-1.88731300	-0.08704200
Mo	1.89813400	0.00172300	-1.68925600
Se	4.12447800	1.61958500	1.45048700
Se	4.13819200	-1.60819900	1.44437300
Mo	5.00974000	0.01277100	-0.32210200
Se	7.05701200	1.89990800	2.75841700
Se	7.07249600	-1.86843300	2.75131200
Mo	7.98414600	0.02221300	1.31659500
Se	2.42678700	0.00844700	-4.19287300
Se	3.90711400	1.62246000	-1.96472100
Se	3.92053700	-1.60038400	-1.97009800
Mo	4.93820200	0.01879300	-3.72384600
Se	6.97206500	1.63489200	-0.44755100
Se	6.98565200	-1.59245200	-0.45368000
Mo	7.73890900	0.02772600	-2.33797200
Se	10.05032100	0.02734400	2.85827300
Se	5.24119300	0.02525200	-6.28770700
Se	6.63790100	1.91015900	-3.64607700
Se	6.65273700	-1.85899500	-3.65232100
Mo	7.34504300	0.03068900	-5.06650900
Se	9.64340000	0.03131700	-0.62976500
Se	9.59194000	0.03813100	-4.13513100

(iii)[MoSe₂]H_{Se}

Mo	-0.27824100	0.00970200	0.01745000
Se	-0.26556500	-0.04677000	2.45044500
Mo	2.08732100	0.00535400	1.42116700
Se	2.93408300	0.03846000	3.82876200
Mo	5.36808100	0.00973200	3.04228700

Se	5.95443200	-0.09375900	5.53407100
Mo	7.90515000	0.00701500	4.08946400
Se	-0.57477900	-0.04184400	-2.39885600
Se	1.30018200	1.89151000	-0.07904100
Se	1.29659100	-1.87516900	-0.08755600
Mo	1.88734200	0.01371400	-1.68108100
Se	4.11749800	1.62359100	1.44257800
Se	4.13149000	-1.59243800	1.42407300
Mo	5.03105000	0.02751600	-0.32478800
Se	7.04212100	1.90383700	2.77293000
Se	7.04886800	-1.86681000	2.74148600
Mo	7.97062300	0.03515300	1.34722400
Se	2.41603100	0.06787500	-4.18207400
Se	3.90088300	1.63163200	-1.95294200
Se	3.91326600	-1.58179400	-1.95238700
Mo	4.92159200	0.02494400	-3.71649300
Se	6.97511300	1.67627400	-0.44736900
Se	7.04416300	-1.57548500	-0.45847200
Mo	7.72169000	0.04005600	-2.36627900
Se	10.00868800	-0.14791000	2.83242900
Se	5.18977000	-0.08638100	-6.26729500
Se	6.62132600	1.91641000	-3.65625100
Se	6.62458800	-1.85464700	-3.64116900
Mo	7.30391800	0.02429100	-5.07830700
Se	9.73968000	0.35111000	-0.63527300
Se	9.54947400	-0.16040200	-4.10473400
H	10.39448800	-0.96829700	-0.67167000

(iv) [MoSe₂]H_{Se}

Mo	-0.27801200	0.00342900	0.01799600
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Se	-0.27574900	-0.00718000	2.44857600
Mo	2.09073000	0.00203000	1.41931300
Se	2.93408800	-0.00027400	3.82691000
Mo	5.36615600	0.00476700	3.04204300
Se	5.95945200	-0.03511500	5.54641000
Mo	7.90273700	-0.00254100	4.09641700
Se	-0.58693100	-0.00053300	-2.39324800
Se	1.29771400	1.89465600	-0.08032000
Se	1.29904600	-1.88694600	-0.08639000
Mo	1.89070800	0.00718700	-1.68001200
Se	4.12114900	1.61593900	1.44060000
Se	4.13106900	-1.60209300	1.42777800
Mo	5.03595900	0.01383000	-0.32558900
Se	7.04273200	1.90342600	2.77851200
Se	7.04957900	-1.87863400	2.73994500
Mo	7.97355700	0.03117500	1.35224600
Se	2.41381600	0.01327900	-4.17908700
Se	3.90358900	1.62006600	-1.95553300
Se	3.91334100	-1.59473300	-1.95503200
Mo	4.92036700	0.01581400	-3.71785500
Se	6.98850200	1.66614900	-0.44884300
Se	7.05687600	-1.58197100	-0.45944700
Mo	7.72305800	0.03797300	-2.37226700
Se	10.01546900	-0.06549500	2.85641900
Se	5.19061400	-0.01923600	-6.28131600
Se	6.61918100	1.91461900	-3.66480400
Se	6.63029300	-1.86826900	-3.63827000
Mo	7.30011800	0.01241800	-5.08621000
Se	9.74449200	0.29386900	-0.63417900
Se	9.55475000	-0.05279800	-4.13082000
H	10.35247000	-1.04833700	-0.66161300

(v) TS1

Mo	5.21357800	-0.84673400	-0.00113800
Se	5.01144600	-3.26403300	-0.03183000
Mo	2.72508100	-2.03260500	-0.01408500
Se	1.66846900	-4.34407800	-0.05759400
Mo	-0.70590300	-3.32779400	-0.01849200
Se	-1.55266500	-5.75155200	0.03720600
Mo	-3.33440700	-4.08478600	-0.03086500
Se	5.78489300	1.50859300	-0.00718000
Se	3.65726300	-0.58097100	-1.88382400
Se	3.65360400	-0.60548500	1.88060500
Mo	3.22204700	1.06270200	0.01257700
Se	0.69350600	-1.83530300	-1.61718500
Se	0.69913300	-1.86729600	1.59682400
Mo	-0.00635700	-0.00329800	0.00869500
Se	-2.36362600	-2.82807000	-1.90768500
Se	-2.35397900	-2.88551100	1.88298500
Mo	-3.09123200	-1.32620900	0.00735200
Se	2.95755000	3.58466100	0.07376600
Se	1.23951600	1.53589500	-1.59007900
Se	1.24174500	1.51931600	1.62884600
Mo	0.38133000	3.37157900	0.02398400
Se	-1.94171600	0.33704700	-1.62032200
Se	-1.93436500	0.29128900	1.65100300
Mo	-2.51158700	2.24320900	0.03765700
Se	-5.30492000	-2.69266300	0.05444300
Se	0.37443500	5.93785600	-0.10399100
Se	-1.32772700	3.48434800	-1.87088600
Se	-1.34083100	3.44822300	1.93086200
Mo	-1.84587500	4.94421400	0.05126900
Se	-4.64706200	0.67358000	-0.06986700
Se	-4.15401400	4.28054400	-0.10289400
H	-4.02267500	1.81109900	1.07905300

(vi) [MoSe₂]H_{Mo}

Mo	-0.24340400	-0.01756000	-0.00064000
Se	-0.27509600	0.07304300	2.42651700
Mo	2.11551400	-0.00044100	1.42078500
Se	2.94288300	0.00712300	3.82789200
Mo	5.40186500	0.01161300	3.03712200
Se	6.01596200	0.03332600	5.53096600
Mo	7.95447800	0.04249100	4.04065500
Se	-0.59152600	0.13162300	-2.38842200
Se	1.31901400	1.87617400	-0.09613500
Se	1.34565600	-1.88284500	-0.10989400

Mo	1.92883200	-0.00523700	-1.71264100
Se	4.15526500	1.59652100	1.41406300
Se	4.14966000	-1.62056200	1.45566500
Mo	5.02958500	-0.03733300	-0.33716600
Se	7.08496700	1.90482800	2.69816600
Se	7.09905700	-1.87132200	2.76002500
Mo	7.97867600	0.00090000	1.26834400
Se	2.37260400	-0.20044700	-4.19540700
Se	3.94147500	1.59697100	-1.96515600
Se	3.92814600	-1.64479200	-1.97728200
Mo	4.91584300	0.00470000	-3.73447000
Se	6.98011100	1.59061400	-0.50436400
Se	6.98966600	-1.67393600	-0.44234400
Mo	7.70093700	-0.08003500	-2.36386200
Se	10.06208800	-0.00042000	2.89019900
Se	5.11312000	0.31815300	-6.26969500
Se	6.66671600	1.87625500	-3.71217000
Se	6.60803500	-1.92183300	-3.68938500
Mo	7.24709100	-0.05337400	-5.13689800
Se	9.64093900	0.11768300	-0.56113100
Se	9.48342000	0.19926900	-4.31456700
H	8.83719000	-1.37382700	-2.42119200

(vii) [MoSe₂]H_{Mo}H_{Se}

Mo	-0.26023000	-0.02654400	0.00641200
Se	-0.29417800	0.01574700	2.45065900
Mo	2.06587600	0.00034900	1.46553600
Se	2.89118200	0.06833800	3.90874400
Mo	5.31118700	0.02692000	3.14320900
Se	5.92082800	-0.13433600	5.64445900
Mo	7.85677100	0.05563800	4.19975800
Se	-0.53415000	0.05112700	-2.39531200
Se	1.30072300	1.86923600	-0.06606900
Se	1.33360400	-1.89084400	-0.06793000
Mo	1.94876400	-0.01206600	-1.65267800
Se	4.09141100	1.61656300	1.49880300
Se	4.10979500	-1.59884700	1.52235500
Mo	5.03950500	-0.00446800	-0.23072300
Se	6.99060500	1.91208700	2.84684400

Se	6.98690900	-1.84412200	2.90436700
Mo	7.93056600	0.01888600	1.45925900
Se	2.47168200	-0.15169100	-4.11676800
Se	3.95598200	1.61046700	-1.88224400
Se	3.97420000	-1.62458400	-1.88399600
Mo	5.00874600	0.02274000	-3.61272800
Se	6.95634400	1.65441600	-0.34968400
Se	7.03093500	-1.62825800	-0.29896600
Mo	7.76238600	-0.02187700	-2.19970100
Se	9.94156700	-0.35400000	2.98017400
Se	5.22983000	0.31325800	-6.12840600
Se	6.73105600	1.91966100	-3.57300200
Se	6.72200700	-1.88841400	-3.52254600
Mo	7.35657000	-0.01736300	-4.97055800
Se	9.73683100	0.48372100	-0.40669800
Se	9.56727300	0.28777000	-4.10802800
H	8.92002500	-1.29078400	-2.23434600
H	10.51574300	-0.76078000	-0.28431000

(viii) TS2

Mo	5.39045000	0.10875300	0.07553700
Se	5.54515500	-2.32860700	0.19804200
Mo	3.15439600	-1.48718200	-0.05089000
Se	2.50584400	-3.97400300	-0.30685000
Mo	0.04425200	-3.36343100	-0.24277600
Se	-0.39009000	-5.89251300	-0.10812400
Mo	-2.41545700	-4.60129000	-0.39120600
Se	5.47611300	2.53344800	0.24752000
Se	3.88596200	0.13467200	-1.85908400
Se	3.74657500	0.03440600	1.89853400
Mo	3.08836100	1.62381100	0.04095900

Se	1.20482300	-1.61091800	-1.76477100
Se	1.07472900	-1.71960400	1.47078000
Mo	0.10062600	0.00402700	-0.12805700
Se	-1.58756600	-3.13489000	-2.18020900
Se	-1.70331900	-3.32413600	1.58398700
Mo	-2.67775500	-1.87501700	-0.27853600
Se	2.34116800	4.05690700	0.08244500
Se	1.11925100	1.76709000	-1.65630600
Se	0.99576500	1.68701000	1.56465300
Mo	-0.13832100	3.37090800	-0.06003800
Se	-1.77377700	0.04509900	-1.82752300
Se	-1.92640400	-0.10875300	1.41667500
Mo	-2.82267100	1.77596400	-0.13569400
Se	-4.58142100	-3.51935400	0.08068300
Se	-0.55183700	5.86658600	-0.29993800
Se	-1.78619400	3.21393000	-1.99138200
Se	-1.89157900	3.14845300	1.78514000
Mo	-2.59654600	4.55651600	-0.09013100
Se	-4.60683100	-0.16864700	-0.90756100
Se	-4.72882200	3.56723100	-0.56304300
H	-4.17402500	1.66254100	1.12894300
H	-4.27647300	1.34619300	2.00310200
O	-4.55448100	0.95165700	3.18249900
H	-4.51385900	-0.06714300	3.24959100
H	-5.44138500	1.23593300	3.43785200
O	-4.36369800	-1.59642800	3.42856100
H	-3.47721300	-1.76344200	3.83025800
H	-4.43532000	-2.17798800	2.66043000
O	-1.84243200	-1.77960000	4.42243800
H	-1.59658900	-2.28476700	5.20259200
H	-1.44132900	-0.89407500	4.53214100

O	-0.77274500	0.78519900	4.49145700
H	-0.05374500	0.98111600	3.87435000
H	-0.64431000	1.38051600	5.23649700
H	-5.52354000	-0.34982300	0.23473500

(ix) [MoSe₂]HSe⁺

Mo	-0.27153400	0.06097300	0.01427700
Se	-0.21775500	-0.23733900	2.44025000
Mo	2.09645100	0.03844600	1.42110500
Se	2.95125100	0.21738500	3.85087000
Mo	5.34769200	0.02780700	3.01413000
Se	5.99169200	-0.26019500	5.48321700
Mo	7.91468900	0.00831600	4.03665400
Se	-0.52142800	-0.25412700	-2.39634700
Se	1.32100200	1.92176700	-0.08538900
Se	1.28298700	-1.83900900	-0.08225000
Mo	1.90099000	0.04034700	-1.68078300
Se	4.10614300	1.68545900	1.44821100
Se	4.11469900	-1.56054300	1.40572300
Mo	5.00346100	0.08580300	-0.32280500
Se	7.03632600	1.89604200	2.73353400
Se	7.00785900	-1.86435500	2.73449600
Mo	7.94005500	0.01922900	1.29856700
Se	2.43037900	0.24017100	-4.19993600
Se	3.89044100	1.69000900	-1.95878100
Se	3.90299300	-1.55623200	-1.92925800
Mo	4.91058800	0.03667600	-3.68264600
Se	6.93768900	1.71573600	-0.44461400
Se	6.96500500	-1.57275700	-0.45294200
Mo	7.70394400	0.02718100	-2.31318900

Se	9.95543500	-0.45750500	2.73337900
Se	5.23074900	-0.23801500	-6.21619700
Se	6.62070500	1.90604100	-3.61636800
Se	6.59373600	-1.85616400	-3.62485500
Mo	7.32405800	0.02176000	-5.02652600
Se	9.73674000	0.56402400	-0.63311700
Se	9.51495100	-0.44496800	-3.99865700
H	10.55892200	-0.65549100	-0.70742000

2. Hydrogen Evolution Reaction (HER) on Pt-MoSe₂:

(i) [Pt-MoSe₂]

Mo	5.15296200	0.54880100	0.22943600
Se	5.46678600	-1.85904600	0.07107100
Pt	2.92463800	-1.23338800	-0.19830500
Se	2.49170300	-3.82834600	-0.12519000
Mo	0.05101400	-3.32485800	-0.02649100
Se	-0.15900900	-5.96890000	0.00006100
Mo	-2.30368400	-4.77945100	0.06972200
Se	5.17225700	2.97272300	-0.13938400
Se	3.81919200	0.43491400	-1.93054400
Se	3.71334300	0.71803000	2.20570300
Mo	2.76624200	1.81400500	0.03497100
Se	0.92826700	-1.56331500	-1.76212100
Se	1.09832600	-1.56243600	1.63882300
Mo	-0.11262800	-0.00478100	-0.00486300
Se	-1.72317600	-3.40175900	-1.92460400
Se	-1.58926800	-3.34466300	1.97874200

Mo	-2.76719100	-2.05983500	0.04830100
Se	1.88817700	4.24218700	0.01723100
Se	0.74947100	1.77041200	-1.66719900
Se	0.70187000	1.78667200	1.65548900
Mo	-0.53316400	3.36197400	-0.02331600
Se	-2.10044400	-0.16706700	-1.63808600
Se	-2.05201300	-0.13510900	1.67718700
Mo	-3.09340100	1.61619100	0.00303000
Se	-4.60906200	-3.92429400	0.10157300
Se	-1.19066000	5.89525100	-0.06739700
Se	-2.21786000	3.07322500	-1.96407700
Se	-2.22317400	3.13022700	1.92497400
Mo	-3.12098100	4.37535900	-0.04036000
Se	-4.74838000	-0.41187700	0.09052000
Se	-5.23301900	3.06120900	-0.04660400

(ii) [Pt-MoSe₂]⁻

Mo	0.54189600	0.28872900	-0.42645800
Se	0.04870900	-0.08111600	1.95635300
Pt	2.62313900	-0.01298300	1.77822900
Se	4.14589800	2.04348000	2.76978600
Mo	5.20573400	0.23694800	4.24323300
Se	6.71180600	2.14611900	5.24554200
Mo	7.12248500	-0.08997500	6.19723700
Se	-0.34370300	2.02970500	-1.64438200
Se	2.75021500	-0.70152000	-0.71872300
Se	-0.59413900	-1.80889400	-1.04653400
Mo	1.11250500	-2.39079600	0.92518500
Se	4.99079800	-0.86541200	1.89993500
Se	2.65660800	-0.27358100	4.28218000

Mo	3.48323700	-2.48208900	3.23357500
Se	7.43075500	-1.12666800	3.95445700
Se	4.71640100	-0.45278800	6.72821500
Mo	5.86721300	-2.48294200	5.55075600
Se	-0.15158400	-4.55731800	0.72834000
Se	3.36087600	-3.54032400	0.83436100
Se	0.92158200	-2.91465900	3.41046700
Mo	1.83315700	-5.03527700	2.25311200
Se	5.68586000	-3.82603000	3.31202800
Se	3.37092100	-3.25442800	5.69182000
Mo	4.03478000	-5.45566800	4.47431700
Se	7.76675500	-2.18075700	7.33115000
Se	0.90728700	-7.54713900	1.70358200
Se	4.13380400	-6.39334000	2.02678200
Se	1.42415700	-5.73802100	4.76809600
Mo	2.53435200	-7.55327300	3.51907800
Se	5.90441000	-5.01990500	6.20717600
Se	4.21382000	-8.02872100	5.20644200

(iii) [Pt-MoSe₂]H_{Se}

Mo	-0.02055000	0.04979700	0.45486600
Se	0.45033600	1.34326400	2.43614800
Pt	2.49902000	-0.06116500	1.91939700
Se	4.79142600	2.45957200	2.65728800
Mo	5.66288300	0.48307600	4.04547300
Se	7.39001800	2.28420700	4.91081800
Mo	7.78956000	0.04053900	5.78263800
Se	-1.11530400	1.28989800	-1.12379000
Se	2.07855800	-0.87177200	-0.50677600
Se	-1.35000400	-1.81619900	1.14433700

Mo	1.19530100	-2.58258500	1.31559900
Se	4.96764800	-0.73818800	1.78866600
Se	3.10639800	0.00456300	4.35637700
Mo	3.73946400	-2.34935400	3.38036400
Se	7.70922700	-1.03575000	3.52999200
Se	5.42719800	-0.10404100	6.58240100
Mo	6.32895700	-2.25715100	5.40293300
Se	0.32288600	-4.87676700	0.87272000
Se	3.48262900	-3.64519900	1.12573700
Se	1.17772100	-2.72698200	3.79759600
Mo	1.97512900	-5.00794000	2.80006900
Se	5.89582200	-3.74556700	3.31183700
Se	3.83648600	-2.90567800	5.88459700
Mo	4.32914500	-5.23486800	4.79523400
Se	8.43458100	-2.00812800	6.94003400
Se	0.74011400	-7.44933400	2.85130200
Se	4.16429600	-6.43446300	2.46889600
Se	1.80601500	-5.42306300	5.41911800
Mo	2.73302100	-7.39512900	4.24466800
Se	6.38069100	-4.70997200	6.24996600
Se	4.53486700	-7.67878200	5.84259300
H	5.65979300	3.60135100	3.08579100

(iv) [Pt-MoSe₂]H_{Se}

Mo	0.00275300	-0.03795000	0.13293700
Se	-0.06455000	0.06978000	2.51548200
Pt	2.45428500	0.08684500	1.80635600
Se	3.09390300	2.04376900	3.83392700
Mo	5.13995100	0.20572300	4.28159900
Se	5.87156400	1.85064500	6.11748300

Mo	7.30730600	-0.17461100	5.91709100
Se	-1.52417900	1.25247900	-1.02220300
Se	2.24430500	0.70935200	-0.68181500
Se	-0.31544400	-2.36773400	-0.57784500
Mo	2.13474900	-1.86673000	-0.32480200
Se	4.96500500	0.47631000	1.67908700
Se	3.01282100	-1.26367500	3.87294800
Mo	4.51017000	-2.03951200	1.89213700
Se	7.63841900	0.27427600	3.47353000
Se	5.32792900	-1.69332200	6.08511000
Mo	6.99701100	-2.20485300	4.10718800
Se	2.45101900	-3.54540200	-2.23703200
Se	4.65606400	-1.78566400	-0.71934900
Se	2.40301700	-3.50434700	1.52073200
Mo	3.99955800	-4.29658700	-0.40282700
Se	7.05032000	-2.26057300	1.50092700
Se	5.04120600	-3.87954600	3.63196200
Mo	6.35081000	-4.78077000	1.57663800
Se	8.89534400	-2.05421900	5.89810400
Se	3.82414000	-6.54284300	-1.94316700
Se	6.54889700	-4.33530200	-1.00245300
Se	4.15441100	-6.19210000	1.48894500
Mo	5.70826700	-6.58553700	-0.40280200
Se	8.12128900	-4.47024700	3.43531400
Se	7.56470000	-7.09656600	1.08877900
H	3.92251800	3.07115200	3.12445100

(v) TS3

Mo	0.11584100	0.32864700	0.05067700
Se	0.06310900	0.46590100	2.48494800

Mo	2.48292100	0.18321600	1.44621400
Se	3.29572600	0.17079700	3.87819200
Mo	5.77232700	-0.05532700	3.03898000
Se	6.39584800	-0.04839100	5.56566800
Mo	8.33818800	-0.24634300	4.07856600
Se	-0.22180000	0.40542900	-2.35900300
Se	1.80017400	2.14397400	-0.13666400
Se	1.44243500	-1.76341100	0.04111100
Mo	2.38084200	0.00065800	-1.64820100
Se	4.60847500	1.67681200	1.45470900
Se	4.33714500	-1.66739700	1.58995200
Mo	5.31274300	-0.13945400	-0.24219900
Se	7.60338200	1.74604900	2.75084700
Se	7.29626800	-2.16212700	2.83116200
Mo	8.33735700	-0.32502900	1.31676900
Se	2.37666700	-0.69668600	-4.06931500
Se	4.42858900	1.61922500	-1.93064400
Se	4.10120300	-1.97265000	-1.68329800
Mo	4.82018700	-0.29087000	-3.46930500
Se	7.39976100	1.41046000	-0.40286100
Se	7.15166700	-1.92918200	-0.38737200
Pt	7.47261600	-0.24163300	-2.28929400
Se	10.45585100	-0.23932900	2.76975600
Se	7.87853200	-0.43482700	-7.26397900
Se	4.87281500	1.20032700	-5.50688200
Se	6.70062000	-2.01704500	-3.98433000
Mo	7.06051700	0.14596900	-5.18403800
Se	10.18841100	-0.56165200	-0.69553400
Se	8.42315600	1.59294900	-3.84723100
H	9.87147600	-1.93752900	-1.18652900

(vi) [Pt-MoSe₂]H_{Pt}

Mo	0.05075800	-0.04228100	-0.17750500
Se	-0.06778700	-0.18065100	2.22384700
Pt	2.50045500	-0.03914000	1.68566900
Se	3.26284900	-0.47850700	4.08955600
Mo	5.16671500	-1.85491600	3.23315400
Se	5.69507400	-1.92898900	5.86761500
Mo	7.31437900	-3.11843800	4.48130200
Se	-1.74450200	1.10905700	-1.04325800
Se	2.13008600	1.21515300	-0.64266100
Se	0.16465900	-2.27319300	-1.08404700
Mo	2.48011600	-1.18370300	-1.50375200
Se	5.03121900	-0.02538200	1.36531200
Se	3.13838500	-2.66435300	1.71437000
Mo	4.94537500	-2.22094400	-0.10866100
Se	7.65901700	-1.18671900	2.93900500
Se	5.52030900	-4.41310100	3.32398200
Mo	7.41135400	-3.50392400	1.75810600
Se	2.51050100	-1.27175800	-3.96380900
Se	4.87694300	-0.36130800	-1.88560200
Se	3.14275200	-3.60637700	-1.34207100
Mo	4.60213700	-2.59217600	-3.20597000
Se	7.48414800	-1.82213100	-0.24847500
Se	5.75654800	-4.65731700	0.14237500
Mo	7.17007300	-3.86057900	-1.88430100
Se	9.14875000	-4.41960500	3.49064900
Se	4.69272900	-3.22554900	-5.80216900
Se	7.07438500	-1.81436000	-3.50124200
Se	5.24347700	-5.18514400	-3.03108700
Mo	6.70906900	-3.97517700	-4.62211000

Se	8.89865000	-4.60909700	-0.06816700
Se	8.67905300	-5.09167700	-3.65880700
H	2.36472700	1.49777000	2.08862800

(vii) [Pt-MoSe₂]H_{Pt}H_{Se}

Mo	0.00521200	0.02868800	-0.01689600
Se	0.00896800	0.20600900	2.36352000
Pt	2.57522700	0.03641000	1.68379600
Se	3.23341900	-0.29182000	4.14448200
Mo	5.26351600	-1.88448700	3.26581200
Se	5.87707100	-1.71089900	5.76168900
Mo	7.41205300	-3.18464500	4.46745400
Se	-1.79728400	1.07886800	-0.95055200
Se	2.12234000	1.11949200	-0.69325400
Se	0.06140800	-2.32391900	-0.54959000
Mo	2.30479500	-1.36972500	-1.38332600
Se	5.09472700	-0.13127600	1.32129400
Se	3.06960600	-2.64672100	1.92976900
Mo	4.79551400	-2.42072500	-0.00679600
Se	7.74820900	-1.34245500	2.79526600
Se	5.47393000	-4.43120700	3.47559400
Mo	7.30991400	-3.69085900	1.77418800
Se	2.12225900	-1.65510400	-3.80296800
Se	4.72281000	-0.65888900	-1.85633800
Se	2.88594500	-3.80124200	-1.08521900
Mo	4.27323800	-2.89759800	-3.07315500
Se	7.33438200	-2.12319400	-0.32461300
Se	5.53705400	-4.87202400	0.31222800
Mo	6.85423100	-4.20209600	-1.83605900
Se	9.09228900	-4.63096500	3.36349600
Se	4.28068400	-3.56281300	-5.67484700
Se	6.78593600	-2.23540300	-3.56966500
Se	4.80497300	-5.50137600	-2.83262900
Mo	6.25466100	-4.44348100	-4.51808900
Se	8.62709200	-4.96526600	-0.15004600
Se	8.27211300	-5.51888800	-3.65966500
H	2.55988900	1.61272000	1.92930300
H	4.03607600	0.95977400	4.30559800

(viii) TS4

Mo	-0.30072000	0.18160100	-0.00249800
Se	-0.36377900	0.06322300	2.44444300

Mo	2.05551500	0.11928900	1.39269300
Se	2.89694400	0.10884400	3.83039400
Mo	5.37247400	0.08627200	2.95261700
Se	6.03022300	0.04112800	5.44282100
Mo	7.94769400	0.08307300	3.89469600
Se	-0.56622300	0.34956600	-2.42497300
Se	1.18666100	2.13853200	-0.04137000
Se	1.19645100	-1.75781200	-0.22293000
Mo	2.04019400	0.23234200	-1.72584900
Se	4.09067600	1.75373200	1.45566400
Se	4.04540100	-1.57793600	1.41590500
Mo	4.84464000	0.08228700	-0.37302100
Se	7.11431400	1.98439100	2.49065600
Se	7.00458300	-1.88193900	2.65332500
Mo	7.91510100	-0.02012600	1.12027500
Se	2.27849000	0.21710300	-4.24330000
Se	3.84385800	2.10085000	-1.69093700
Se	3.80056000	-1.66818000	-1.94897300
Mo	4.56380600	0.35110900	-3.30714500
Se	6.96269700	1.50695300	-0.90103900
Se	6.88605800	-1.67216800	-0.64367600
Pt	8.03358400	-0.25874100	-2.46044600
Se	10.01456600	-0.36431900	2.58665500
Se	7.21442800	0.63745200	-7.38438000
Se	5.36203500	2.48648700	-4.55297800
Se	6.27992000	-1.33897000	-4.18427700
Mo	7.00810600	0.82276900	-5.12159500
Se	9.89405200	0.15848000	-0.70270700
Se	9.10486200	1.46322300	-4.14440000
H	9.02277100	-1.44469900	-3.29085800
H	9.14569900	-2.37126100	-3.15165600
O	9.34558900	-3.63767800	-2.94412800
H	9.81277500	-3.66083800	-2.04533800
H	9.96770300	-3.96763800	-3.61450200
O	10.34039100	-3.36968000	-0.53409600
H	9.72409400	-3.77171300	0.14319000
H	11.23322900	-3.62987400	-0.26616500
O	8.66021600	-4.47198000	1.24960500
H	8.88398800	-5.34078300	1.61027200
H	7.69723300	-4.52042400	1.05370400
O	5.91419900	-4.73076800	0.80867300
H	5.27981000	-4.58041300	1.52455100
H	5.48340600	-4.38004100	0.01535900
H	10.31134400	-1.27588100	-0.52675600

(ix) [Pt-MoSe₂]H_{Se}⁺

Mo	-0.00284400	0.02452100	-0.28957400
Se	0.12940000	-1.44474700	1.61757300
Pt	2.49320500	-0.72416500	1.03530700

Se	3.50848900	-0.43426000	4.40770800
Mo	5.43827100	-1.72348900	3.33311500
Se	6.40982000	-1.67279700	5.79007100
Mo	7.85243100	-2.83388100	4.21385000
Se	-1.72784500	1.51717100	-0.33634000
Se	2.10365000	1.33475000	-0.47841500
Se	-0.15260600	-1.43844200	-2.25360000
Mo	2.24180300	-0.84666600	-1.84308900
Se	4.92205300	0.00853300	1.40173800
Se	3.43615400	-2.83191000	2.03777800
Mo	4.84190800	-2.09184300	-0.05233000
Se	7.79599100	-0.93136100	2.60121000
Se	5.96527800	-4.26165200	3.42655300
Mo	7.48403500	-3.29714700	1.53398000
Se	2.63484100	-0.98932300	-4.32429200
Se	4.74931200	-0.27741100	-1.95397500
Se	2.82490600	-3.20311200	-1.27311600
Mo	4.34765700	-2.51555600	-3.28238100
Se	7.32592800	-1.71379200	-0.53671300
Se	5.62160300	-4.52302400	0.14929600
Mo	6.85910400	-3.82239000	-2.05108800
Se	9.51470500	-4.10999700	2.92885300
Se	4.23202900	-3.37680900	-5.84961800
Se	6.79873700	-1.87161900	-3.78330100
Se	4.79237800	-5.09617100	-2.96009700
Mo	6.25170400	-4.10625100	-4.71068500
Se	8.73649800	-4.48447500	-0.40364900
Se	8.19372900	-5.27292500	-3.75181600
H	3.93747600	-0.31176600	5.83264700

3. Pt-MoSe₂ for Oxygen Reduction Reaction (ORR).

(i) [Pt-MoSe₂]

Mo	5.15296200	0.54880100	0.22943600
Se	5.46678600	-1.85904600	0.07107100
Pt	2.92463800	-1.23338800	-0.19830500
Se	2.49170300	-3.82834600	-0.12519000
Mo	0.05101400	-3.32485800	-0.02649100

Se	-0.15900900	-5.96890000	0.00006100
Mo	-2.30368400	-4.77945100	0.06972200
Se	5.17225700	2.97272300	-0.13938400
Se	3.81919200	0.43491400	-1.93054400
Se	3.71334300	0.71803000	2.20570300
Mo	2.76624200	1.81400500	0.03497100
Se	0.92826700	-1.56331500	-1.76212100
Se	1.09832600	-1.56243600	1.63882300
Mo	-0.11262800	-0.00478100	-0.00486300
Se	-1.72317600	-3.40175900	-1.92460400
Se	-1.58926800	-3.34466300	1.97874200
Mo	-2.76719100	-2.05983500	0.04830100
Se	1.88817700	4.24218700	0.01723100
Se	0.74947100	1.77041200	-1.66719900
Se	0.70187000	1.78667200	1.65548900
Mo	-0.53316400	3.36197400	-0.02331600
Se	-2.10044400	-0.16706700	-1.63808600
Se	-2.05201300	-0.13510900	1.67718700
Mo	-3.09340100	1.61619100	0.00303000
Se	-4.60906200	-3.92429400	0.10157300
Se	-1.19066000	5.89525100	-0.06739700
Se	-2.21786000	3.07322500	-1.96407700
Se	-2.22317400	3.13022700	1.92497400
Mo	-3.12098100	4.37535900	-0.04036000
Se	-4.74838000	-0.41187700	0.09052000
Se	-5.23301900	3.06120900	-0.04660400

(ii) [O₂_Pt-MoSe₂]

Mo	-0.06690200	-0.49054100	0.04412200
Se	-0.07225600	-0.51646500	2.46558100
Pt	2.34232900	-0.15342900	1.55844200
Se	3.08344000	-0.48523400	4.07224200

Mo	5.40770800	-0.83469400	3.24679300
Se	5.91288700	-1.21567200	5.82597300
Mo	7.88824200	-1.32638700	4.38055700
Se	-0.25887800	0.34783700	-2.37657300
Se	1.27831100	1.69710100	0.19300200
Se	1.05159300	-2.48866100	-0.63565600
Mo	2.08283000	-0.13484300	-1.51057900
Se	4.50343900	1.16434600	1.79938200
Se	3.95911000	-2.18946000	1.48490500
Mo	5.17306100	-0.51008600	-0.03499500
Se	7.36994400	0.86254400	3.30553700
Se	6.80931400	-2.97250900	2.85045900
Mo	8.04056100	-1.02859200	1.64523100
Se	2.70142700	0.03179000	-4.02917300
Se	4.23043000	1.38989200	-1.50672200
Se	4.01644000	-1.87770400	-1.86954400
Mo	5.19791900	-0.13691800	-3.41792300
Se	7.31769300	0.91804100	0.04715000
Se	6.94735800	-2.34485800	-0.33480400
Mo	7.93998600	-0.56529700	-2.00652900
Se	10.06281600	-1.49526900	3.22523400
Se	5.57669000	0.19249200	-5.99473200
Se	7.07262400	1.61666000	-3.11093700
Se	6.72986600	-2.21360000	-3.60193500
Mo	7.64797300	-0.19014400	-4.72809600
Se	9.80714100	-1.02166800	-0.25206700
Se	9.89019500	-0.49185800	-3.72261300
O	6.33161400	4.20078300	1.09671100
O	5.85402500	4.13492000	-0.02150300

(iii) [2O_Pt-MoSe₂]

Mo	0.01446400	0.10414000	-0.15080900
Se	-0.11194600	0.20034500	2.20705700
Pt	2.37412600	0.09066900	1.50676200
Se	3.13080500	0.59686900	3.93141600
Mo	5.26998000	1.80142900	3.31047400
Se	5.75027200	1.76633900	5.90897700
Mo	7.57761800	2.71443400	4.57835800
Se	-1.87205400	-0.54864500	-1.26856900
Se	0.35985800	2.54508200	-0.64578800
Se	2.00620800	-1.21762400	-0.77590300
Mo	2.64721600	1.22872700	-1.33129000
Se	3.46758900	3.06764800	1.80804200
Se	4.87914100	0.03623500	1.40646000
Mo	5.10114000	2.17503500	-0.07108800
Se	5.97851500	4.28008800	3.47658900
Se	7.62941600	0.79866500	2.99585500
Mo	7.67085400	3.14071600	1.85475800
Se	2.46902800	1.53460000	-3.82044500

Se	3.38067600	3.66340600	-1.28640600
Se	4.91321500	0.22468000	-1.77529200
Mo	4.72694600	2.43584500	-3.11782200
Se	6.15038700	4.50015800	0.23324400
Se	7.57763500	1.48509200	-0.17065600
Mo	7.45373600	3.52139700	-1.80243700
Se	9.49268500	3.89867000	3.50672400
Se	5.00829300	2.92625200	-5.76956300
Se	5.60421500	4.95747400	-2.97453700
Se	7.19361500	1.49020700	-3.42441600
Mo	6.98477600	3.66514700	-4.53481800
Se	9.23793400	4.13114700	-0.06428300
Se	9.09020000	4.53132200	-3.66409900
O	3.68861300	4.77783600	1.86309500
O	0.95134000	3.28798000	0.82428900

(iv) [2O_Pt-MoSe₂]

Mo	0.02484600	0.09766200	-0.16225200
Se	-0.11421000	0.20047100	2.19761900
Pt	2.38174100	0.10433700	1.51502100
Se	3.13745000	0.60469300	3.94224400
Mo	5.28886700	1.81657900	3.32039100
Se	5.76382100	1.76764700	5.92124000
Mo	7.59286900	2.70985300	4.56867300
Se	-1.84119600	-0.58904900	-1.31992100
Se	0.35193200	2.54234000	-0.66473400
Se	2.02846600	-1.22124000	-0.76223800
Mo	2.64497000	1.22377800	-1.33364200
Se	3.47964100	3.08083900	1.83403400
Se	4.88813800	0.04842900	1.42158900
Mo	5.09351400	2.18052900	-0.06691100
Se	6.02512900	4.31071900	3.48130000
Se	7.66072500	0.78458300	2.99525100
Mo	7.66587200	3.12991900	1.83019200
Se	2.46344300	1.53251800	-3.82436500
Se	3.37538100	3.66328900	-1.28256100
Se	4.92051700	0.23635800	-1.77173900
Mo	4.72476100	2.44087000	-3.11665000
Se	6.13998200	4.52094600	0.24370100
Se	7.57223800	1.46550400	-0.17589300
Mo	7.41672800	3.50667900	-1.79550700
Se	9.54229800	3.79891900	3.53801100
Se	4.99314300	2.92729200	-5.77797100
Se	5.59682000	4.99198600	-2.97155000
Se	7.21230300	1.47857800	-3.44912100
Mo	6.96196100	3.67107500	-4.52665400
Se	9.21082400	4.14212900	-0.03384900
Se	9.07251200	4.51748500	-3.67014700
O	3.67678100	4.80091200	1.85156700

O	0.84422700	3.32473300	0.80874800
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(v) [OH_O_Pt-MoSe₂]

Mo	-0.00303700	0.00654400	-0.00240300
Se	-0.00649700	-0.00527200	2.42633000
Pt	2.38931500	-0.00781200	1.45800600
Se	3.43444600	0.79156800	3.64355000
Mo	5.74588400	1.34272300	2.71238100
Se	6.40859900	1.64812700	5.23912000
Mo	8.28812200	1.89527900	3.67116600
Se	-0.38176900	0.10293700	-2.42251300
Se	1.02166100	2.33418400	-0.22013100
Se	1.70193400	-1.80500200	-0.32280700
Mo	2.13114100	0.41371600	-1.64480300
Se	4.13807200	2.72396600	1.11936400
Se	4.82288700	-0.61477900	1.21381100
Mo	5.26211900	1.12606000	-0.63456100
Se	6.99733700	3.58743900	2.37677100
Se	7.78957100	-0.22916600	2.47798400
Mo	8.18720900	1.81498200	0.91186000
Se	2.51195700	0.36928000	-4.24781000
Se	3.73689300	2.45204200	-2.19024500
Se	4.43513300	-0.83427000	-2.05038200
Mo	4.98084800	0.92730400	-3.91840300
Se	6.84528100	3.19086600	-0.87286000
Se	7.50976400	-0.10265000	-0.75944200
Mo	7.77856900	1.55803200	-2.75479000
Se	10.31505300	2.33407100	2.32363600
Se	5.11618800	0.83248700	-6.54346000
Se	6.25158000	3.17721900	-4.09202800
Se	7.04513900	-0.63113800	-3.95444000
Mo	7.25310400	1.34888800	-5.45609500
Se	9.73939300	2.14779700	-1.14760100
Se	9.55444200	1.76740900	-4.62649700
O	-0.00037500	3.33223000	-1.45394000
O	4.92369900	4.21284600	0.54792500
H	0.00311000	2.84891900	-2.30229000

(vi) TS5

Mo	0.03423400	0.21334300	0.14102700
Se	0.09704400	-0.11306800	2.55039400
Pt	2.44665900	-0.04368900	1.48467900
Se	3.49535800	0.70424200	3.68457300
Mo	5.77210500	1.30888500	2.72863900
Se	6.45290700	1.60126400	5.25975200
Mo	8.31677800	1.87175600	3.68343300
Se	-0.44535600	0.46486400	-2.31817300

Se	0.98740000	2.43601800	-0.27963800
Se	1.58784800	-1.71279000	-0.36547700
Mo	2.12678300	0.51882700	-1.58673300
Se	4.13404900	2.70453500	1.16964300
Se	4.86659800	-0.66521700	1.22354700
Mo	5.25969800	1.11912200	-0.59995300
Se	7.00900700	3.56466200	2.40811900
Se	7.82549800	-0.25045600	2.48385200
Mo	8.20448900	1.80594500	0.92766600
Se	2.47333600	0.44078700	-4.19674900
Se	3.77786900	2.50371200	-2.14389300
Se	4.39835200	-0.80221800	-2.03411900
Mo	4.95992100	0.96408500	-3.89289700
Se	6.84828400	3.18516000	-0.83898000
Se	7.51078800	-0.10120100	-0.74741100
Mo	7.77250400	1.56245100	-2.73863000
Se	10.33624000	2.32886600	2.32326700
Se	5.07728000	0.87434000	-6.51635300
Se	6.26370900	3.20009300	-4.07098200
Se	7.00708700	-0.61637400	-3.93564400
Mo	7.23040200	1.35835500	-5.44023300
Se	9.74120800	2.15144400	-1.15118600
Se	9.53873300	1.75513300	-4.62806400
O	-0.36137600	2.64645500	-2.07631000
O	4.91765000	4.19863000	0.59719800
H	0.06498600	3.07698500	-2.84881600

(vii) [O_Pt-MoSe₂]

Mo	-0.08066200	0.24941300	-0.06822800
Se	-0.41393900	-0.29256200	2.27595200
Pt	2.10545700	-0.54441600	1.46467600
Se	3.10648400	-0.40970300	3.85424500
Mo	5.52662600	-0.69202400	3.18114700
Se	5.99468500	-0.93514900	5.77384500
Mo	7.97366800	-1.27448700	4.36314300
Se	-0.23137800	0.74815700	-2.42864700
Se	1.75276900	1.87472300	0.36965300
Se	1.04268300	-1.96225900	-0.46854200
Mo	2.22085700	0.13493800	-1.50390900
Se	4.78169200	1.38053400	1.70776100
Se	4.12251700	-2.05505300	1.42581700
Mo	5.28460700	-0.40061500	-0.15614300
Se	7.57138500	0.91878400	3.26206700
Se	6.85326500	-2.90303000	2.86400500
Mo	8.12701200	-1.00472900	1.61600600
Se	2.81913300	0.29721100	-4.00978200
Se	4.46939300	1.54318400	-1.60323100
Se	4.00646200	-1.77496600	-1.90071100

Mo	5.30241500	-0.11920700	-3.46258100
Se	7.53310300	0.95307800	-0.02647300
Se	6.97019900	-2.33379000	-0.34241300
Mo	8.00422700	-0.68124900	-2.08285900
Se	10.14694400	-1.48599000	3.19336000
Se	5.64380200	0.05526100	-6.05179800
Se	7.27989900	1.53030200	-3.23603900
Se	6.68183800	-2.30438800	-3.62237000
Mo	7.71735900	-0.36153600	-4.80305600
Se	9.87789600	-1.03513700	-0.30240500
Se	9.92429900	-0.89768500	-3.79583900
O	6.16235500	2.45986100	1.38418600

(vii) [O_Pt-MoSe₂]-

Mo	0.01061000	0.00915800	-0.00979300
Se	-0.04956000	0.00609000	2.41477200
Pt	2.43070800	-0.01818900	1.37638000
Se	3.60357600	0.88649600	3.50150100
Mo	5.96706900	0.88173600	2.59046000
Se	6.69391800	1.36875100	5.09631600
Mo	8.56116300	1.03295000	3.52696400
Se	-0.48731600	-0.11072800	-2.36862700
Se	1.51848800	1.97521000	-0.19479800
Se	1.49951800	-2.01560800	-0.05511000
Mo	2.15006000	-0.06392000	-1.68058900
Se	4.70834600	2.34599000	0.77257000
Se	4.71525200	-1.09256400	1.38527200
Mo	5.39470400	0.27961600	-0.68108500
Se	7.65851300	2.81374400	2.04903000
Se	7.68034000	-1.09605600	2.59753500
Mo	8.38169200	0.65448500	0.78873900
Se	2.44887800	-0.41309800	-4.22133700
Se	4.06335000	1.64088600	-2.39315000
Se	4.24021900	-1.67481500	-1.87316400
Mo	5.00416100	-0.25853700	-3.93693100
Se	7.28565700	2.06661600	-1.12902000
Se	7.39859300	-1.33084500	-0.64288300
Mo	7.84400600	0.02811600	-2.83270500
Se	10.61015800	0.90949700	2.16727400
Se	5.05615000	-0.67110000	-6.53546800
Se	6.62705300	1.74116500	-4.37193000
Se	6.80009500	-2.15815800	-3.78736300
Mo	7.26763700	-0.39361000	-5.49502200
Se	9.89978800	0.49844300	-1.32293600
Se	9.60822400	-0.21623400	-4.76070500
O	5.82015200	3.51609700	-0.02296800

(viii) [OH_Pt-MoSe₂]

Mo	0.08396700	-0.02097800	-0.14102300
Se	0.02560100	-0.00835400	2.27522300
Pt	2.57182200	-0.00429400	1.26704500
Se	3.55823000	0.76471100	3.58677500
Mo	5.95573900	0.72633900	2.72910800
Se	6.66793500	1.15397000	5.21257800
Mo	8.56326100	0.84023200	3.65509500
Se	-0.43127000	-0.10474800	-2.47893100
Se	1.58645800	1.91931600	-0.35403500
Se	1.60070200	-1.96659300	-0.20699100
Mo	2.40093500	-0.06393300	-1.90006800
Se	4.63210000	2.27013600	1.02533900
Se	4.71537100	-1.25287700	1.54695900
Mo	5.30750200	0.21894200	-0.47720300
Se	7.69137900	2.61390300	2.15589000
Se	7.65514800	-1.27716000	2.72598900
Mo	8.38574900	0.44371100	0.91431200
Se	2.38577300	-0.40180300	-4.35828500
Se	4.15767400	1.76038600	-2.24668600
Se	4.28295300	-1.79210400	-1.75408100
Mo	4.86022300	-0.23541000	-3.69110900
Se	7.27273400	1.82441400	-1.00539800
Se	7.30771400	-1.46002600	-0.52162400
Mo	7.80761800	-0.08026800	-2.68185300
Se	10.60430600	0.65698900	2.29032600
Se	5.02763500	-0.57647200	-6.37528600
Se	6.62384600	1.68797700	-4.22326300
Se	6.66913800	-2.21025800	-3.71511500
Mo	7.23439400	-0.43408700	-5.34044000
Se	9.90340200	0.16686400	-1.17210600
Se	9.56338700	-0.32475400	-4.66105700
O	5.69773800	3.73848300	0.37111200
H	5.29859000	4.53083300	0.77368300

(ix) TS6

Mo	-0.01621600	-0.01680600	-0.02151900
Se	-0.02200800	0.00465400	2.40249400
Pt	2.36740800	0.01376600	1.44863200
Se	3.31209800	0.99653200	3.61119400
Mo	5.53620000	1.67451900	2.60007600
Se	6.10167200	2.33758900	5.09498300
Mo	8.00789600	2.51437800	3.55805300
Se	-0.35019500	-0.42027200	-2.48823700
Se	0.76663100	2.18350100	-0.87746600
Se	1.67593500	-1.89951100	-0.19385900
Mo	2.10328700	0.14241700	-1.74852500
Se	3.76421900	2.67130000	0.84095500

Se	4.81881500	-0.53652300	1.34403700
Mo	5.19467300	1.03783200	-0.64818500
Se	6.67555100	3.93264700	2.01403400
Se	7.67764100	0.22009500	2.64978500
Mo	8.03914200	2.05475900	0.83466400
Se	2.57222300	-0.17931800	-4.30401300
Se	3.70763100	2.12753700	-2.41981100
Se	4.46585600	-1.07189700	-1.89833700
Mo	5.02056400	0.46770100	-3.94444100
Se	6.65567900	3.08103200	-1.13383800
Se	7.51074900	-0.08119300	-0.60180600
Mo	7.76563400	1.36470700	-2.77693300
Se	10.07009100	2.88098200	2.25967000
Se	5.25455900	0.09404400	-6.53774500
Se	6.21712800	2.72952800	-4.36104400
Se	7.15370800	-0.98026700	-3.71125500
Mo	7.33975400	0.79229000	-5.44857200
Se	9.67713400	2.12985800	-1.16734600
Se	9.56634200	1.52363100	-4.63207400
O	4.00183300	4.42125900	0.12233000
H	4.83893200	4.80419300	0.44502300