Supplementary Information

Nanostructured Pt-Doped 2D MoSe$_2$: An Efficient Bifunctional Electrocatalyst for both Hydrogen Evolution and Oxygen Reduction Reactions

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Periodic Calculations:

1. 2D Monolayer Pristine MoSe$_2$:

```
  _chemical_name_common                 'BG_MoSe2'
  _cell_length_a                      3.234700
  _cell_length_b                      3.234700
  _cell_length_c                       20.00000
  _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'
```
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
| Atom Site Label | Occupancy | Fract X   | Fract Y   | Fract Z   |
|----------------|-----------|-----------|-----------|-----------|
| 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  |
Finite Non-periodic Molecular Cluster Model Systems with their Equilibrium Structures

1. Hydrogen Evolution Reaction (HER) on MoSe₂:

(i) [MoSe₂]

|   | X    | Y    | Z    |
|---|------|------|------|
| 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]-

|   | X    | Y    | Z    |
|---|------|------|------|
| 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 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| 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<sub>se</sub>

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| 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   |
| Element | x          | y          | z          |
|---------|------------|------------|------------|
| 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      | 3.90083300 | 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) $\text{[MoSe}_2\text{]}_\text{HSe}$

| Element | x          | y          | z          |
|---------|------------|------------|------------|
| Mo      | -0.27801200| 0.00342900 | 0.01799600 |
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  -1.68001200   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      10.19061400  -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

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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      | -3.34407000| -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      | -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 | -0.10399100|
| 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| 0.05443300|
| 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]H₂Mo

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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|
(vii) $[\text{MoSe}_2]H\text{Mo}H\text{Se}$

|     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|
| 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  | 4.91584300  | 0.00470000  | -3.73447000 |
| Mo  | 6.98011100  | 1.59061400  | -0.50436400 |
| Se  | 7.70093700  | -0.08003500 | -2.36386200 |
| Mo  | 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  | 7.85677100  | 0.05563800  | 4.19975800  |
| Se  | 5.92082800  | -0.13433600 | 5.64459000  |
| Mo  | 7.85677100  | 0.05563800  | 4.19975800  |
| Se  | -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 | 5.64459000  |
| 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  |
| Element | x     | y     | z     |
|---------|-------|-------|-------|
| 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 |
| 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

| Element | x     | y     | z     |
|---------|-------|-------|-------|
| 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| 1.204823 | -1.610918 | -1.764771 |
| Se| 1.074729 | -1.719604 | 1.470780  |
| Mo| 0.100626 | 0.004027 | -0.128057 |
| Se| -1.587566 | -3.134890 | -2.180209 |
| Se| -1.703319 | -3.324136 | 1.583987  |
| Mo| -2.677755 | -1.875017 | -0.278536 |
| Se| 2.341168 | 4.056907 | 0.082445  |
| Se| 1.119251 | 1.767090 | -1.656306 |
| Se| 0.995765 | 1.687010 | 1.564653  |
| Mo| -0.138321 | 3.370908 | -0.060038 |
| Se| -1.773777 | 0.045099 | -1.827523 |
| Se| -1.926404 | -0.108753 | 1.416675 |
| Mo| -2.822671 | 1.775964 | -0.135694 |
| Se| -4.581421 | -3.519354 | 0.080683  |
| Se| -0.551837 | 5.866586 | -0.299938 |
| Se| -1.786194 | 3.213930 | -1.991382 |
| Se| -1.891579 | 3.148453 | 1.785140  |
| Mo| -2.596546 | 4.556516 | -0.090131 |
| Se| -4.606831 | -0.168647 | -0.907561 |
| Se| -4.728822 | 3.567231 | -0.563043 |
| H | -4.174025 | 1.662541 | 1.128943  |
| H | -4.276473 | 1.346193 | 2.003102  |
| O | -4.554481 | 0.951657 | 3.182499  |
| H | -4.513859 | -0.067143 | 3.249591  |
| H | -5.441385 | 1.235933 | 3.437852  |
| O | -4.363698 | -1.596428 | 3.428561  |
| H | -3.477213 | -1.763442 | 3.830258  |
| H | -4.435320 | -2.177988 | 2.660430  |
| O | -1.842432 | -1.779600 | 4.422438  |
| H | -1.596589 | -2.284767 | 5.202592  |
| H | -1.441329 | -0.894075 | 4.532141  |
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)  \([\text{MoSe}_2]\text{HSe}^+\)

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 -4.19936000
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

S13
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
### (iii) [Pt-MoSe₂]H-Se

| Element | x            | y            | z            |
|---------|--------------|--------------|--------------|
| 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   |
| Element | x     | y     | z     |
|---------|-------|-------|-------|
| 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-MoSe$_2$]H$_{Se}$

| Element | x     | y     | z     |
|---------|-------|-------|-------|
| 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 |
| Element | x          | y          | z          |
|---------|------------|------------|------------|
| 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

| Element | x          | y          | z          |
|---------|------------|------------|------------|
| Mo      | 0.11584100 | 0.32864700 | 0.05067700 |
| Se      | 0.06310900 | 0.46590100 | 2.48494800 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| 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| -0.13664400|
| Se      | 1.44243500| -1.76341100| 0.04111000|
| 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|
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| 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  |
|     | X      | Y      | Z      |
|-----|--------|--------|--------|
| Se  | 8.89865 | -4.609097 | -0.068167 |
| Se  | 8.679053 | -5.091677 | -3.658807 |
| H   | 2.364727 | 1.49777 | 2.088628 |

(vii) \([\text{Pt-MoSe}_2]H_{\text{PtHSe}}\)

|     | X      | Y      | Z      |
|-----|--------|--------|--------|
| Mo  | 0.005212 | 0.028688 | -0.016896 |
| Se  | 0.008968 | 0.206009 | 2.36352 |
| Pt  | 2.575227 | 0.03641 | 1.683796 |
| Se  | 3.233419 | -0.29182 | 4.144482 |
| Mo  | 5.263516 | -1.884487 | 3.265812 |
| Se  | 5.877071 | -1.710899 | 5.761689 |
| Mo  | 7.412053 | -3.184645 | 4.467454 |
| Se  | -1.797284 | 1.078868 | -0.950552 |
| Se  | 2.12234 | 1.119492 | -0.693254 |
| Se  | 0.061408 | -2.323919 | 0.54959 |
| Mo  | 2.304795 | -1.369725 | -1.383326 |
| Se  | 5.094727 | -0.131276 | 1.321294 |
| Se  | 3.069606 | -2.646721 | 1.929769 |
| Mo  | 4.795514 | -2.420725 | -0.006796 |
| Se  | 7.748209 | -1.342455 | 2.795266 |
| Se  | 5.47393 | 4.431207 | 3.475594 |
| Mo  | 7.309914 | 3.690859 | 1.774188 |
| Se  | 2.122259 | 1.655104 | -3.802968 |
| Se  | 4.72281 | 0.658889 | -1.856338 |
| Se  | 2.885945 | -3.801242 | -1.085219 |
| Mo  | 4.273238 | -2.897598 | -3.073155 |
| Se  | 7.334382 | -2.123194 | -0.324613 |
| Se  | 5.537054 | -4.872024 | 0.312228 |
| Mo  | 6.854231 | -4.202096 | -1.836059 |
| Se  | 9.092289 | -4.630965 | 3.363496 |
| Se  | 4.280684 | -3.562813 | -5.67487 |
| Se  | 6.785936 | -2.235403 | -3.569665 |
| Se  | 4.804973 | -5.501376 | -2.832629 |
| Mo  | 6.254661 | -4.443481 | -4.518089 |
| Se  | 8.627092 | -4.965266 | -0.15046 |
| Se  | 8.272113 | -5.518888 | -3.659665 |
| H   | 2.559889 | 1.61272 | 1.929303 |
| H   | 4.036076 | 0.959774 | 4.305598 |

(viii) TS4

|     | X      | Y      | Z      |
|-----|--------|--------|--------|
| Mo  | -0.30072 | 0.181601 | -0.002498 |
| Se  | -0.363779 | 0.063223 | 2.44443 |

S20
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
Se       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  -0.70270700
Se       7.91510100  1.50695300  -0.90103900
Mo       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  -4.14093500
Se       9.10486200  1.46322300  -3.14404000
H        9.02277100 -1.44469900  -3.29085800
H        9.14569900 -2.37126100  -3.15165600
O        9.34558900 -3.63767800   2.49412800
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       10.62016000 -4.47198000   1.24960500
H       10.88398800 -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]²⁺

Mo       -0.00284400  0.02452100  -0.28957400
Se       0.12940000 -1.44474700   1.61753700
Pt       2.49320500  0.72416500   1.03530700
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Se      | 3.50848900 | -0.43426000 | 4.40770800 |
| Mo      | 5.43827100 | -1.72388100 | 3.33311500 |
| Se      | 6.40982200 | -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|
| 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      | 7.95999100 | -0.93136100 | 2.60121000 |
| Se      | 5.96527800 | -4.26165200 | 3.42655300 |
| Mo      | 7.48403500 | -2.97147000 | 1.53398000 |
| Se      | 2.63484100 | -0.98932300 | -4.32429200|
| Se      | 4.74931200 | -0.27741100 | -1.95397500|
| Se      | 2.82490600 | -3.20312000 | -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 | -4.10997000 | 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-MoSe$_2$ for Oxygen Reduction Reaction (ORR).

(i) [Pt-MoSe$_2$]

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Mo      | 5.15296200 | 0.54880100 | 0.22943600 |
| Se      | 5.46678600 | -1.85904600| 0.07107100 |
| Pt      | 2.92463800 | -1.23388000| -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) [O$_2$Pt-MoSe$_2$]

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
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| 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 |
| Mo      | 1.05159300| -2.48866100| -0.63565600|
| Se      | 2.08283000| -0.13484300| -1.51057900|
| Se      | 4.50343900| 1.16434600  | 1.79938200 |
| Mo      | 3.95911000| -2.18946000| 1.48490500 |
| Mo      | 5.17306100| -0.51008600| -0.03499500|
| Se      | 7.36944400| 0.86254400  | 3.30533700 |
| 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-MoSe$_2$]

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| 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|
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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 | 3.89670000 | 3.50672400 |
| Se      | 5.00829300 | 2.92625200 | -5.76956300|
| Se      | 5.60421500 | 4.95747400 | -2.97453700|
| Se      | 7.19361500 | 1.49020700 | -3.42416000|
| 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) \([2O_{\text{Pt-MoSe}_2}]\)

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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 |

(v) [OH_O_Pt-MoSe$_2$]

|   | 0.00303700 | 0.00654400 | -0.00240300 |
| Mo | 2.38931500 | -0.00781200 | 1.45800600 |
| Se | 3.43444600 | 0.79156800 | 3.64355000 |
| Pt | 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 | -0.32280700 |
| Se | 2.13114100 | 0.41371600 | -1.64480300 |
| Se | 4.13807200 | 2.72396600 | 1.11936400 |
| Se | 4.82288700 | -0.61477900 | -3.91840300 |
| Mo | 6.99733700 | 3.58743900 | 2.37677100 |
| Se | 7.78951000 | -0.22916600 | -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 | -0.63133800 | -3.95444000 |
| Mo | 7.25310400 | 1.34888800 | -5.45609500 |
| Se | 9.73939300 | 2.14779700 | -1.14760100 |
| Se | 9.55444200 | 1.76740900 | -4.62497000 |
| O | 0.00375000 | 3.32230000 | -1.45394000 |
| O | 4.92369900 | 4.21284600 | 0.54792500 |
| H | 0.00311000 | 2.84919000 | -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 | 1.30888800 | 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 -2.14393000  
Mo 4.95992100 0.96408500 -3.89289700  
Se 6.84828400 3.18516000 -0.83980000  
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 5.39468500 -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  

S27
|     | x     | y     | z     |
|-----|-------|-------|-------|
| 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  |
| 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) \([O_{Pt-MoSe_2}]^+\)

|     | x     | y     | z     |
|-----|-------|-------|-------|
| 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) \([OH_{Pt-MoSe_2}]^-\)
|   | x         | y         | z         |
|---|-----------|-----------|-----------|
| 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 | -0.19358900 |
| Mo| 2.10328700  | 0.14241700  | -1.74852500 |
| Se| 3.76421900  | 2.67130000  | 0.84095500 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| 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 | -3.9444100 |
| 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 | -6.5374500 |
| 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 |