Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

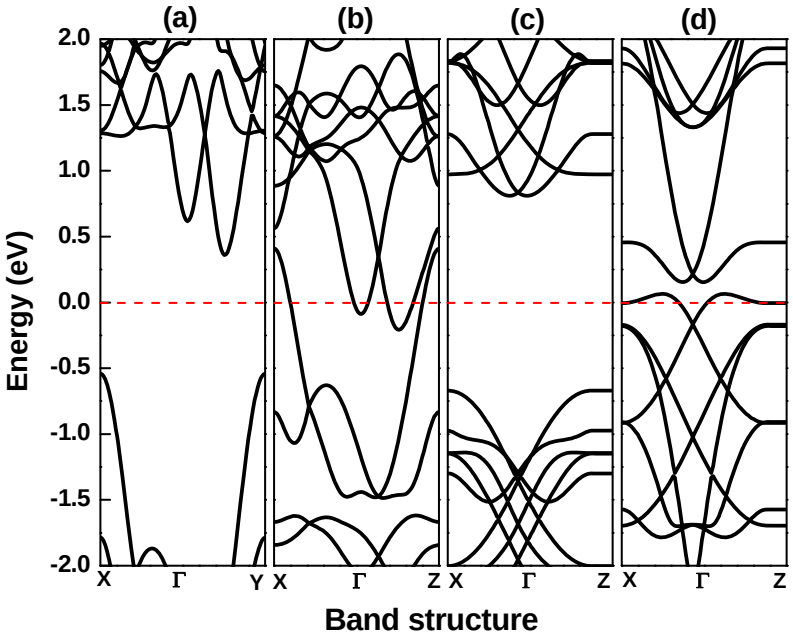

Fig. S1 Band structures of monolayers for (a) MoO_2 with the lattice parameter of a=2.78 Å, which corresponds to the original stable structure. (b) MoO_2 with a=3.24 Å, which is forced to fit the lattice parameter of Janus OMoTe. (c) $MoTe_2$ with a=3.46 Å, which corresponds to the original stable structure. (d) $MoTe_2$ with a=3.24 Å, which is forced to fit the lattice parameter of Janus OMoTe. The original MoO_2 and $MoTe_2$ are semiconductors, see (a) and (c). However, when they are forced to fit the lattice parameter of OMoTe, both of them become metallic, see (b) and (d). The Fermi level is set to be zero.

Table S1 The calculated cohesive energy (E_c) and formation energy (E_f) of monolayer XMoY (X, Y=O, S, Se and Te) per unit. The formulas of the energies come from Ref [Ataca et al., *J. Phys. Chem. C*, 2012, 116, 8983].

	E_{atom}(eV)	E_{bulk}(eV)	E_c^a(eV)	E_f^b(eV)
O	-431.06845	-435.53077	4.46232	
S	-273.22920	-277.32147	4.09227	
Se	-285.04647	-285.37275	0.32628	
Te	-2481.22991	-2484.49008	3.26017	
Mo	-1855.05741	-1866.11995	11.06254	
OMoS	-2559.35506	-2583.17106	23.81600	4.19887
OMoSe	-2571.17233	-2593.75298	22.58065	6.72951
OMoTe	-4767.35577	-4788.26697	20.91120	2.12617
SMoSe	-2413.33308	-2434.35975	21.02667	5.54558
SMoTe	-4609.51652	-4629.28448	19.76796	1.35298
SeMoTe	-4621.33379	-4640.32394	18.99015	4.34116

[a] Corresponding equation: $E_c = E_{atom}[\mathrm{Mo}] + E_{atom}[\mathrm{X}] + E_{atom}[\mathrm{Y}] - E_{atom}[\mathrm{XMoY}]$

[b] Corresponding equation: $E_c = E_c[\mathrm{XMoY}] - E_c[\mathrm{X}] - E_c[\mathrm{Y}] - E_c[\mathrm{Mo}]$, and E_f is obtained by subtracting the cohesive energies of the constituent elements in their equilibrium (bulk, liquid, or gas) phases [Ataca et al., *J. Phys. Chem. C*, 2012, 116, 8983].

Table S2 The bong lengths in MoO2, MoTe2 and OMoTe monolayers.

Structure	Bond Length (Å)
Mo-O bond (MoO2)	2.00
Mo-Te bond (MoTe2)	2.69
Mo-O bond (OMoTe)	2.15
Mo-Te bond (OMoTe)	2.85

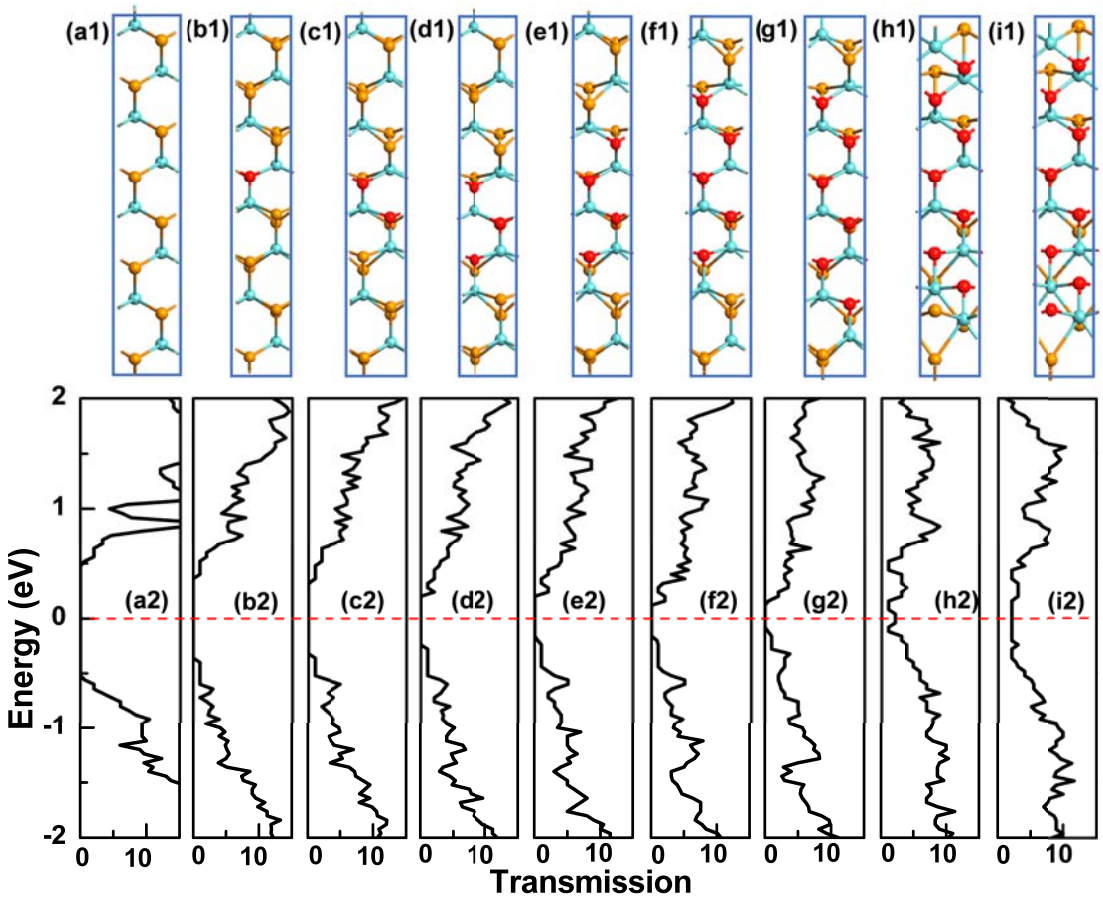

Fig. S2 The geometries (upper panel) and corresponding transmission spectra (lower panel) of $O_{n/8}MoTe_{2-n/8}$ (n=0-8), corresponding to Fig. 4 in the paper.

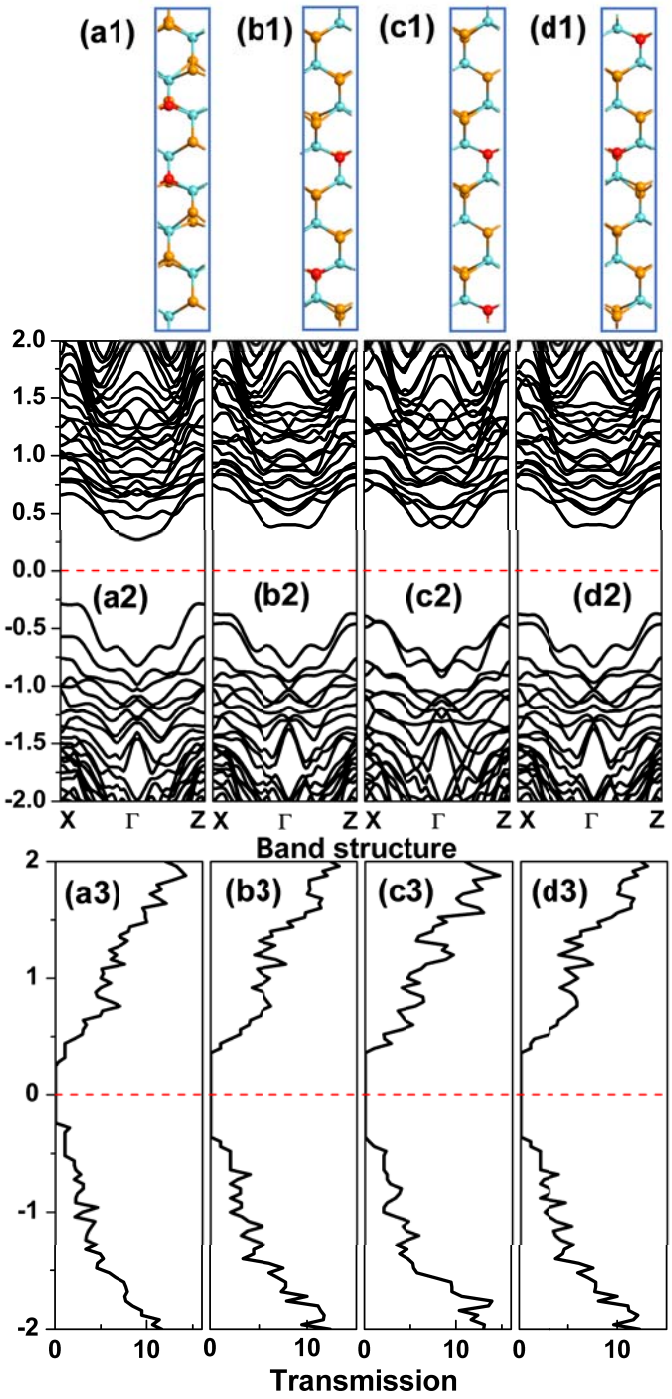

Fig. S3 The geometries (a), band structures (b) and transmission spectra (c) of $O_{2/8}MoTe_{2\text{-}2/8}$-*p* (*p*=1, 2, 3 and 4). They possess the same ratio of O atoms like $O_{2/8}MoTe_{2\text{-}2/8}$ (where the O atoms are adjacent), but with different distributions.

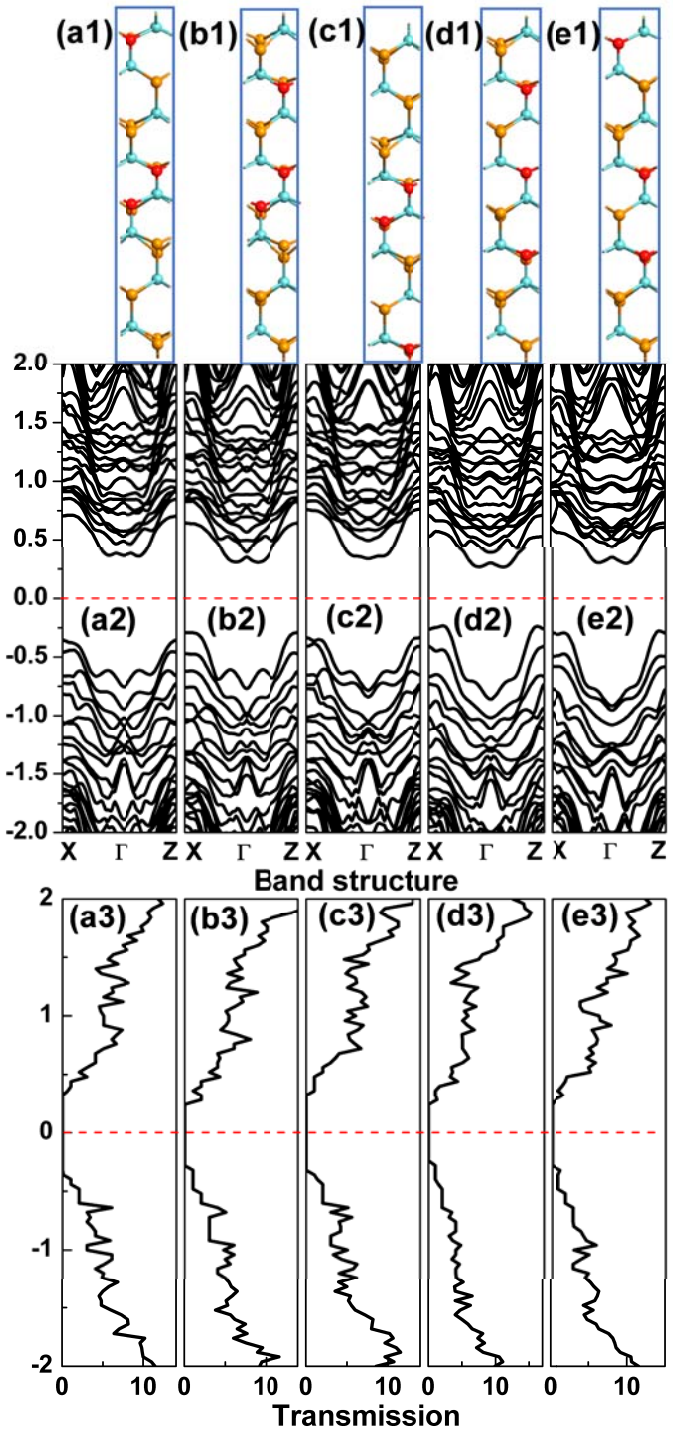

Fig. S4 The geometries (a), band structures (b) and transmission spectra (c) of $O_{3/8}MoTe_{2\text{-}3/8}$-*p* (*p*=1, 2, 3, 4 and 5). They possess the same ratio of O atoms like $O_{3/8}MoTe_{2\text{-}3/8}$ (where the O atoms are adjacent), but with different distributions.

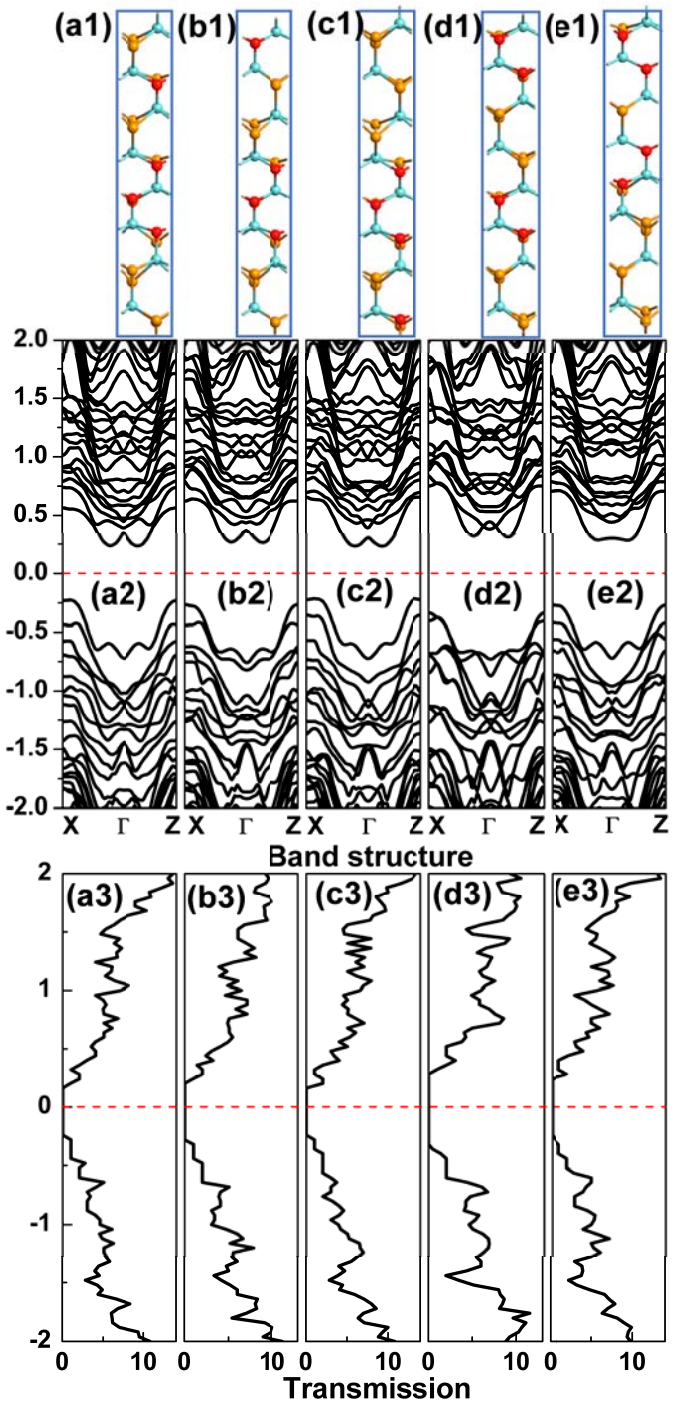

Fig. S5 The geometries (a), band structures (b) and transmission spectra (c) of $O_{4/8}MoTe_{2\text{-}4/8}$-*p* (*p*=1, 2, 3, 4 and 5). They possess the same ratio of O atoms like $O_{4/8}MoTe_{2\text{-}4/8}$ (where the O atoms are adjacent), but with different distributions.

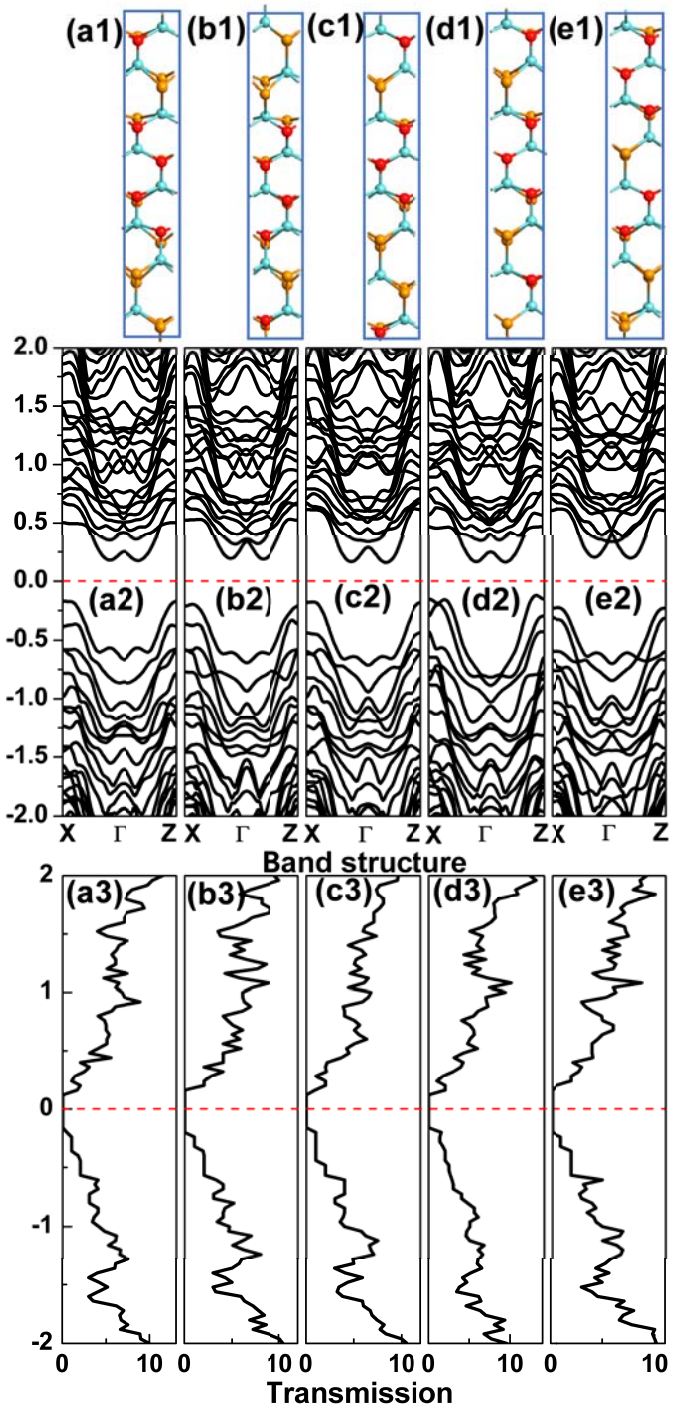

Fig. S6 The geometries (a), band structures (b) and transmission spectra (c) of $O_{5/8}MoTe_{2\text{-}5/8}$-*p* (*p*=1, 2, 3, 4 and 5). They possess the same ratio of O atoms like $O_{5/8}MoTe_{2\text{-}5/8}$ (where the O atoms are adjacent), but with different distributions.

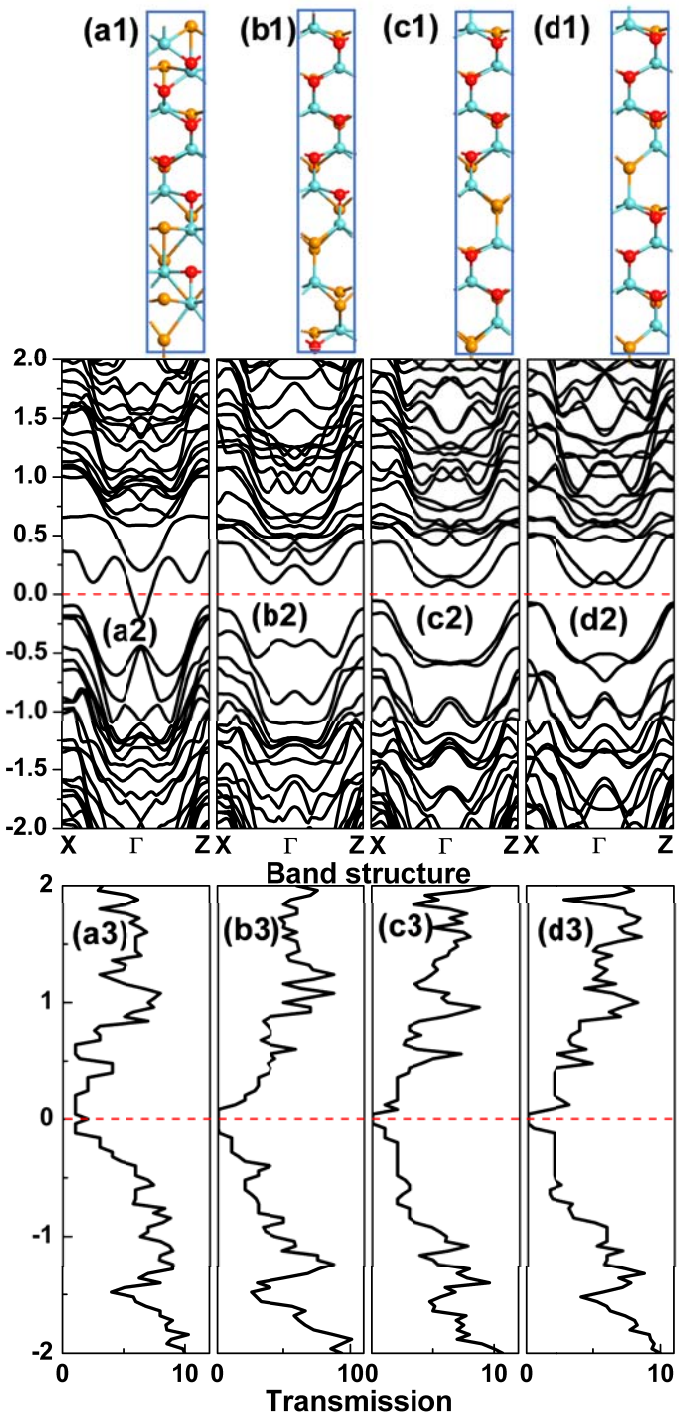

Fig. S7 The geometries (a), band structures (b) and transmission spectra (c) of $O_{6/8}MoTe_{2\text{-}6/8}$-*p* (*p*=1, 2, 3 and 4). They possess the same ratio of O atoms like $O_{6/8}MoTe_{2\text{-}6/8}$ (where the O atoms are adjacent), but with different distributions.

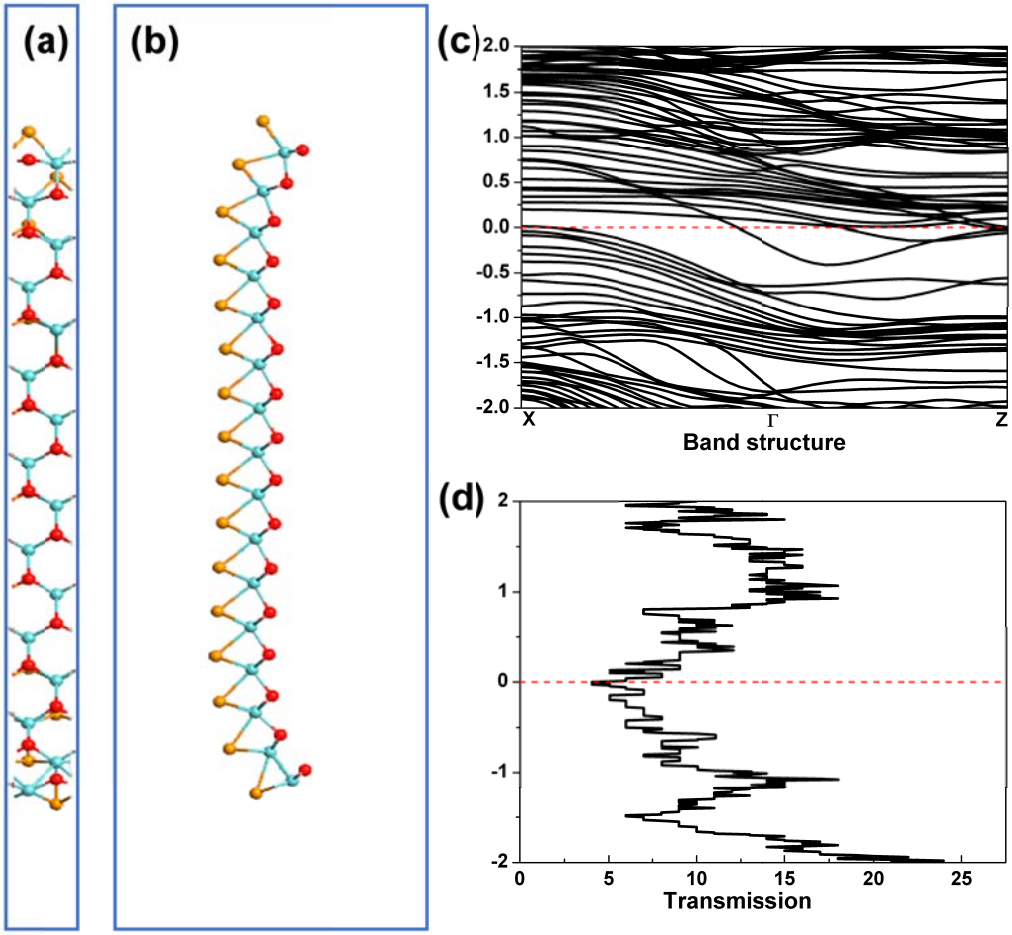

Fig. S8 The geometries (a)-(b), band structure (c) and transmission spectrum (d) of OMoTe-ribbon.

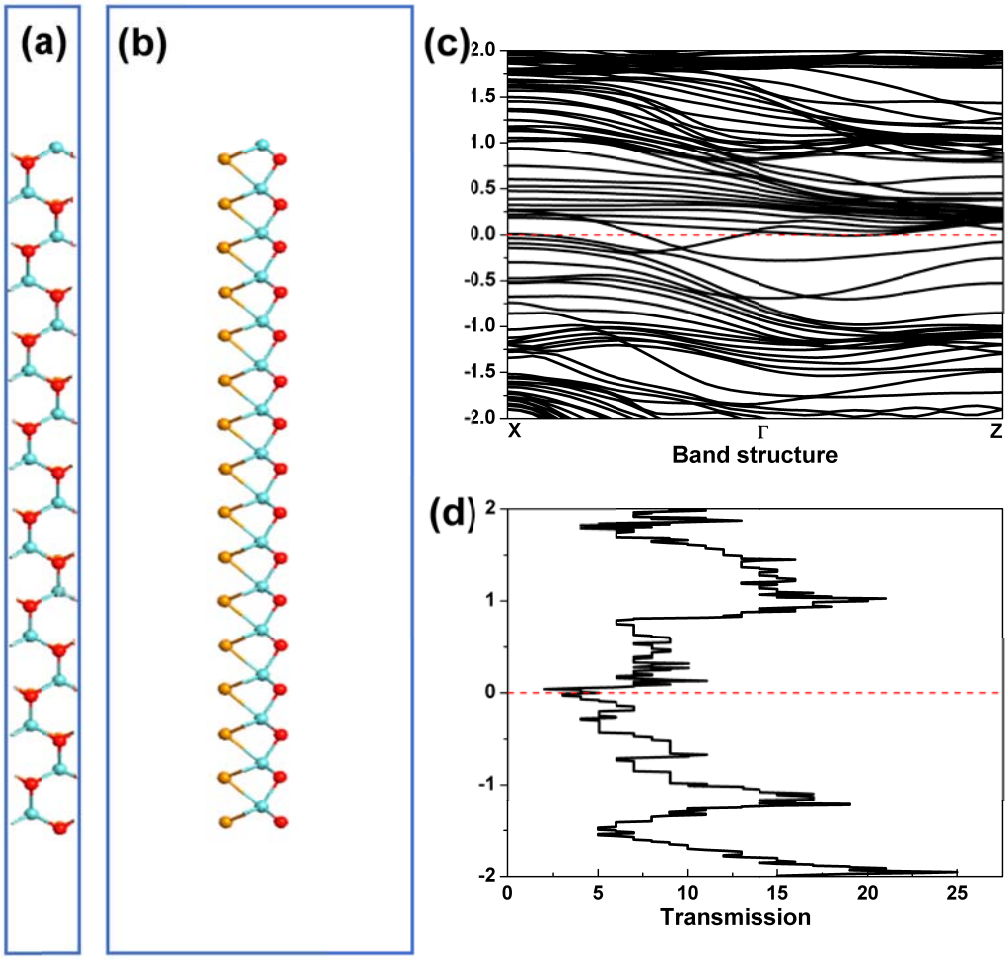

Fig. S9 The geometries (a)-(b), band structure (c) and transmission spectrum (d) of OMoTe-ribbon(unopti). Note the nanoribbon cutting from OMoTe monolayer has not been optimized.

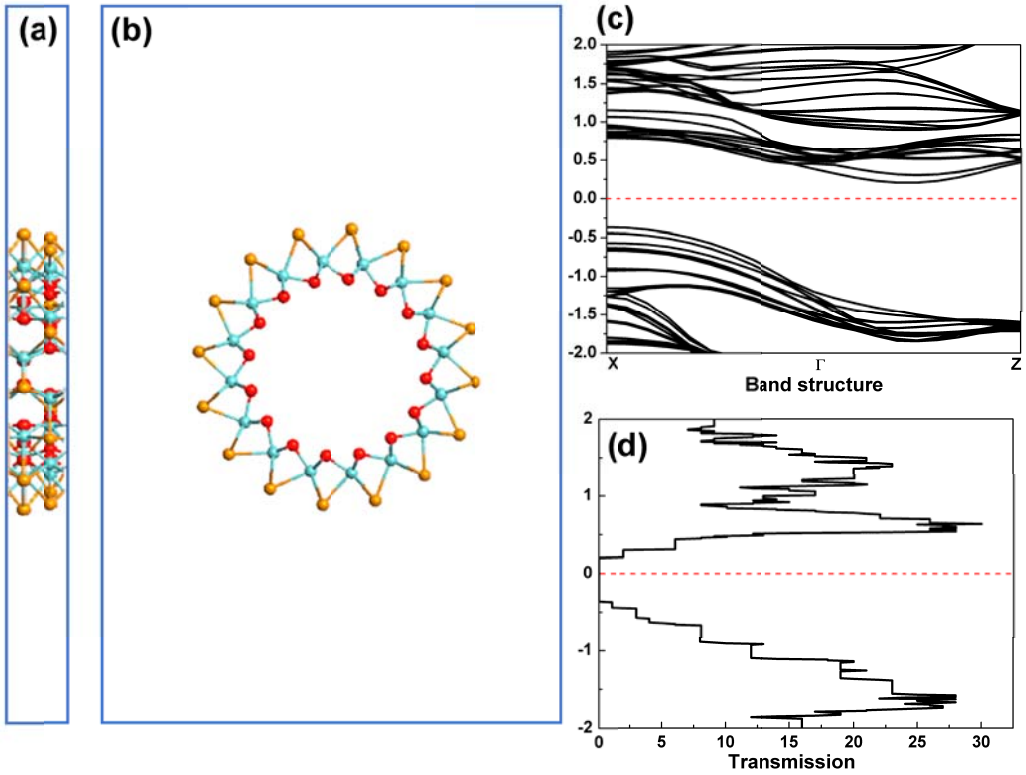

Fig. S10 The geometries (a)-(b), band structure (c) and transmission spectrum (d) of OMoTe-tube.

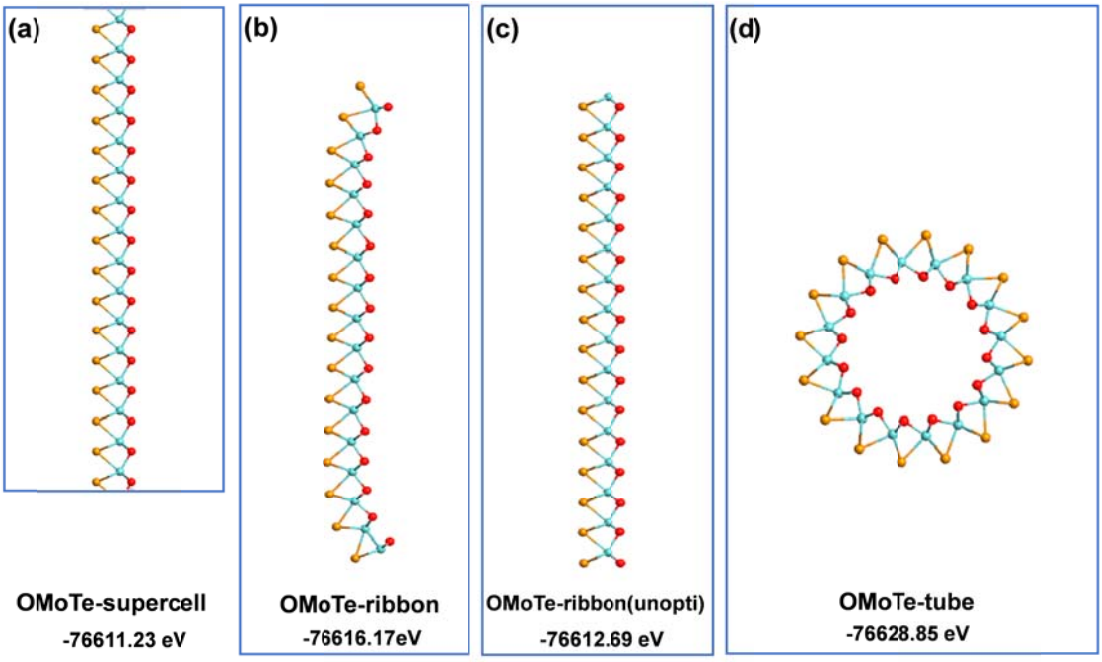

Fig. S11 The geometries of (a) OMoTe-supercell, (b) OMoTe-ribbon, (c) OMoTe-ribbon(unopti) and (d) OMoTe-tube. For each case, the total energy of it is shown at the bottom.

The Cartesian coordinates of the optimized $O_{n/8}MoTe_{2-n/8}$ (or $O_{n/8}MoTe_{2-n/8}$-*p*) configurations, where *p* denotes the other possible configurations with the same number of O atoms (n) in the supercell.

$O_{1/8}MoTe_{2-1/8}$

```
==============================
# Set up lattice
vector_a = [24.1888, 0.0, 0.0]*Angstrom
vector_b = [0.0, 20.012, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.53891]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.084371099641,  0.522594876226,  0.749983913326],
                        [ 0.57607867558 ,  0.473472144644,  0.749994023001],
                        [ 0.341465296622,  0.500361621809,  0.749996839042],
                        [ 0.826367842391,  0.513198402759,  0.749997127084],
                        [ 0.213284250831,  0.515478726179,  0.249982827161],
                        [ 0.697901463354,  0.496318518537,  0.249991823967],
                        [ 0.469995549816,  0.477186895167,  0.249982324182],
                        [ 0.95535571167 ,  0.521775083178,  0.249988357413],
                        [ 0.173617188044,  0.609920966574,  0.749981772521],
                        [ 0.644271852789,  0.582523107252,  0.749991117795],
                        [ 0.438162992018,  0.576949434118,  0.749975520208],
                        [ 0.907917419171,  0.610753989206,  0.74998917198 ],
                        [ 0.040739356707,  0.614366408082,  0.24998501227 ],
                        [ 0.544592266147,  0.520066793839,  0.249999210125],
                        [ 0.306096455961,  0.59707977223 ,  0.249995868232],
                        [ 0.77517798202 ,  0.599122991689,  0.249997491115],
                        [ 0.16640066767 ,  0.426743153106,  0.749980535395],
                        [ 0.667581505421,  0.396987190699,  0.749991761498],
                        [ 0.41525858013 ,  0.39423672149 ,  0.749984678201],
                        [ 0.916149734522,  0.427744262817,  0.74998835338 ],
                        [ 0.041362360035,  0.430981538037,  0.249984561343],
                        [ 0.542333296033,  0.370713629276,  0.249984611709],
                        [ 0.291046491224,  0.414495965883,  0.249997003282],
                        [ 0.791424137194,  0.41681044087 ,  0.249998696799]]
```

$O_{2/8}MoTe_{2-2/8}$

```
==============================
# Set up lattice
vector_a = [23.6502, 0.0, 0.0]*Angstrom
vector_b = [0.0, 20.0684, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.49124]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Tellurium, Tellurium, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.089934989768,  0.53484576705 ,  0.749483989608],
                        [ 0.56785823608 ,  0.470911886669,  0.749350784068],
                        [ 0.353211907973,  0.478494574902,  0.749371364405],
                        [ 0.823988340496,  0.530698052127,  0.74945282033 ],
                        [ 0.221576686141,  0.514333219638,  0.249412553926],
                        [ 0.692388637674,  0.506922007464,  0.249409852939],
                        [ 0.461482040265,  0.455875546769,  0.249370979097],
                        [ 0.956933327762,  0.539815670956,  0.249474963978],
                        [ 0.187728310011,  0.612801428307,  0.74951569943 ],
                        [ 0.630710224607,  0.586570569422,  0.74948646696 ],
                        [ 0.434280800112,  0.509686361884,  0.749443880007],
                        [ 0.907616100774,  0.628882450242,  0.749566294929],
                        [ 0.048050711394,  0.62913135821 ,  0.249585883718],
                        [ 0.528526692835,  0.514961736135,  0.249405455454],
                        [ 0.326128891597,  0.581132768368,  0.249476953355],
                        [ 0.767872739993,  0.613995974903,  0.249533561783],
                        [ 0.166903508314,  0.4312436795  ,  0.749337281527],
                        [ 0.667540449162,  0.405445609376,  0.749300857708],
                        [ 0.414770009806,  0.360911768595,  0.749250234384],
                        [ 0.916240187189,  0.446178426207,  0.749380299984],
                        [ 0.04183898803 ,  0.446241396134,  0.249397215311],
                        [ 0.544561831059,  0.364081594582,  0.249242594161],
                        [ 0.290412242578,  0.402459641903,  0.249290638576],
                        [ 0.791128314916,  0.432883127106,  0.249350718856]]
```

$O_{2/8}MoTe_{2-2/8}$-1

```
==============================
# Set up lattice
vector_a = [23.7239, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9717, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.48813]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Oxygen, Oxygen, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.092613597975,  0.52226886119 ,  0.750212209236],
                        [ 0.571499718416,  0.485053387258,  0.750437466646],
                        [ 0.333820121744,  0.477205882409,  0.750490962702],
                        [ 0.828001490848,  0.531872752326,  0.750215234786],
                        [ 0.225951272407,  0.493776049837,  0.250364216759],
                        [ 0.696246509284,  0.514261026059,  0.250310904997],
                        [ 0.462851269462,  0.476257368222,  0.250497091762],
                        [ 0.960835818829,  0.533657800845,  0.250287382297],
                        [ 0.19417248027 ,  0.595216686251,  0.75022003219 ],
                        [ 0.638093809527,  0.597994735092,  0.750233804245],
                        [ 0.418991158598,  0.572655863186,  0.750439671054],
                        [ 0.915123180323,  0.625819154695,  0.750206317725],
                        [ 0.054830208407,  0.61914260956 ,  0.250159588621],
                        [ 0.535047151337,  0.529048245885,  0.250485232915],
                        [ 0.304871657269,  0.529371462433,  0.250441518078],
                        [ 0.775020224532,  0.618318438576,  0.250158563766],
                        [ 0.1660571859  ,  0.414161703991,  0.750367470318],
                        [ 0.66797453135 ,  0.413520955153,  0.750403547179],
                        [ 0.417038633977,  0.384271466537,  0.750656542917],
                        [ 0.916606803873,  0.441947322629,  0.750353696228],
                        [ 0.041798008578,  0.435526292331,  0.250258110263],
                        [ 0.545371868004,  0.378723138727,  0.250674918901],
                        [ 0.290903523372,  0.379202645097,  0.250409202413],
                        [ 0.791850392882,  0.4352508529  ,  0.250271888573]]
```

$O_{2/8}MoTe_{2-2/8}$-2

```
==============================
# Set up lattice
vector_a = [23.809, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9827, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.49116]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.096236616764,  0.498275457688,  0.750329160388],
                        [ 0.573826303004,  0.494126967339,  0.749988425405],
                        [ 0.330600385143,  0.496791839281,  0.750288133606],
                        [ 0.831612538736,  0.525477455722,  0.750270314827],
                        [ 0.204569565221,  0.488519921216,  0.25030808516 ],
                        [ 0.699397951564,  0.516441243394,  0.250027417668],
                        [ 0.465266916326,  0.491538555801,  0.250147558421],
                        [ 0.963300558951,  0.519035603651,  0.250620874759],
                        [ 0.173207447354,  0.538267584222,  0.750329329175],
                        [ 0.64475698174 ,  0.603127961602,  0.749968274046],
                        [ 0.421923295287,  0.586452875816,  0.750164117113],
                        [ 0.922301885973,  0.613904105972,  0.750621612364],
                        [ 0.061298370231,  0.597990788921,  0.250334865552],
                        [ 0.538535334118,  0.540118857844,  0.250030578393],
                        [ 0.283551370229,  0.589384653804,  0.250291947182],
                        [ 0.782718922866,  0.615046808485,  0.250189886533],
                        [ 0.165877161568,  0.387966081738,  0.750400256148],
                        [ 0.667150527661,  0.417597519631,  0.750034339666],
                        [ 0.416300396706,  0.402331494295,  0.750217563974],
                        [ 0.915802183249,  0.430020010182,  0.750619563874],
                        [ 0.040118422528,  0.415164294806,  0.250352541613],
                        [ 0.543662996249,  0.389636965599,  0.250011237452],
                        [ 0.291319827072,  0.401743790281,  0.250311271533],
                        [ 0.791192209116,  0.431513777618,  0.25025113958 ]]
```

$O_{2/8}MoTe_{2-2/8}$-3

```
==============================
# Set up lattice
vector_a = [23.8463, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9757, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.48662]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium,
            Tellurium, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.076999775274,  0.49523503222 ,  0.750129020227],
                        [ 0.576737764352,  0.495526050157,  0.749886805864],
                        [ 0.334797834664,  0.512218328703,  0.750007592142],
                        [ 0.834820014786,  0.51181599195 ,  0.749896968299],
                        [ 0.203133638002,  0.510180383268,  0.250069557855],
                        [ 0.703159557831,  0.509976235056,  0.249941235832],
                        [ 0.468438145181,  0.498967145029,  0.249939391036],
                        [ 0.968627603024,  0.498246098842,  0.24988858603 ],
                        [ 0.152083151907,  0.60004273012 ,  0.750063087377],
                        [ 0.652208245658,  0.599883787199,  0.749932223826],
                        [ 0.429251126703,  0.596458561975,  0.749973543601],
                        [ 0.929491507659,  0.595828710794,  0.749890878694],
                        [ 0.043827710356,  0.543299863186,  0.250157166711],
                        [ 0.543439384936,  0.543967133622,  0.249854503071],
                        [ 0.289779014606,  0.604474780181,  0.25002036997 ],
                        [ 0.789895050988,  0.604140048031,  0.249902194589],
                        [ 0.16685166553 ,  0.413228370981,  0.750073512152],
                        [ 0.666619242663,  0.413249237508,  0.749938470699],
                        [ 0.415951237122,  0.4125736045  ,  0.749951039132],
                        [ 0.91590463451 ,  0.412066928721,  0.749866033004],
                        [ 0.042418412164,  0.392576880037,  0.250096552143],
                        [ 0.542426560351,  0.392891539598,  0.249897548636],
                        [ 0.291379887515,  0.420190305823,  0.250003152446],
                        [ 0.791296454068,  0.419824024455,  0.249886422495]]
```

$O_{2/8}MoTe_{2-2/8}$-4

```
==============================
# Set up lattice
vector_a = [23.8086, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9817, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.48952]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium,
            Tellurium, Oxygen, Tellurium, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.074126529937,  0.516444031922,  0.750273244272],
                        [ 0.579743236513,  0.488479840971,  0.749881428681],
                        [ 0.338293904528,  0.520227391758,  0.749796683111],
                        [ 0.839913463188,  0.490799831307,  0.750228690787],
                        [ 0.206406543252,  0.525996912655,  0.250024652554],
                        [ 0.705831368508,  0.496376378243,  0.250124691909],
                        [ 0.471410390372,  0.498685292951,  0.249843436607],
                        [ 0.94855646539 ,  0.493713852775,  0.250188827124],
                        [ 0.157225431871,  0.615349657195,  0.7500404114  ],
                        [ 0.658882921086,  0.58909943957 ,  0.750096073445],
                        [ 0.436492708206,  0.598500978444,  0.749777091022],
                        [ 0.913007403053,  0.539613481472,  0.75014825136 ],
                        [ 0.019435135381,  0.603137375917,  0.250291932291],
                        [ 0.548513586602,  0.538368892988,  0.249893994026],
                        [ 0.296972575621,  0.614920391628,  0.249815724874],
                        [ 0.797050869742,  0.586052046481,  0.250261797036],
                        [ 0.166170824791,  0.431813484684,  0.750067812985],
                        [ 0.666247987842,  0.401419273921,  0.750090768696],
                        [ 0.415123145451,  0.415791535422,  0.749825364018],
                        [ 0.918514618756,  0.389205906754,  0.750292804328],
                        [ 0.041976886513,  0.41755458867 ,  0.250290812692],
                        [ 0.540782463594,  0.388078191088,  0.249867850186],
                        [ 0.290886051417,  0.43109219838 ,  0.249813375311],
                        [ 0.791138519196,  0.401419279437,  0.250237244845]]
```

$O_{3/8}MoTe_{2-3/8}$

==========

```
# Set up lattice
vector_a = [23.1694, 0.0, 0.0]*Angstrom
vector_b = [0.0, 20.0585, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.44654]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Tellurium, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.098119010851,  0.534546730154,  0.75178790334 ],
                        [ 0.561762550064,  0.481002468118,  0.751169070045],
                        [ 0.342650731981,  0.457318833105,  0.748827022668],
                        [ 0.824753948371,  0.550030283642,  0.752496279696],
                        [ 0.233447560607,  0.492046900707,  0.250725016927],
                        [ 0.689084915349,  0.524923242597,  0.251698609897],
                        [ 0.454434782125,  0.453977794506,  0.24689995727 ],
                        [ 0.962392423936,  0.552728101641,  0.252760625785],
                        [ 0.207838786727,  0.59637470958 ,  0.751107908449],
                        [ 0.622041604438,  0.60089887195 ,  0.751858977541],
                        [ 0.418713624204,  0.504849753516,  0.745295265988],
                        [ 0.914229823603,  0.644336272052,  0.752834538317],
                        [ 0.062204327179,  0.633301231487,  0.251964191698],
                        [ 0.518146870221,  0.521208400813,  0.249158779813],
                        [ 0.318111394415,  0.515246137409,  0.249423598693],
                        [ 0.766117601748,  0.633191535675,  0.252596505037],
                        [ 0.16549055192 ,  0.420091349999,  0.751137312936],
                        [ 0.667015229468,  0.422336729086,  0.751510285115],
                        [ 0.416372989597,  0.352854481419,  0.748299763261],
                        [ 0.916423161429,  0.461572632411,  0.752663421638],
                        [ 0.042185822635,  0.451319212979,  0.251837249808],
                        [ 0.546649450918,  0.372017434512,  0.25057498471 ],
                        [ 0.286988261536,  0.368309369584,  0.249971543478],
                        [ 0.790689982014,  0.452130288932,  0.252398299213]]
```

$O_{3/8}MoTe_{2-3/8}$-1

```
==============================
# Set up lattice
vector_a = [23.4509, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9384, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.44417]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Oxygen, Tellurium, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.079453523238,  0.529133661277,  0.752033945858],
                        [ 0.570983742575,  0.484767549855,  0.751669233421],
                        [ 0.351753924196,  0.499164721776,  0.750648965724],
                        [ 0.838821448825,  0.508969624758,  0.751290064762],
                        [ 0.214763197399,  0.526029704334,  0.251727446476],
                        [ 0.69989362359 ,  0.506782298627,  0.251086120717],
                        [ 0.462199906711,  0.476379720054,  0.251073297088],
                        [ 0.949736297771,  0.511427645679,  0.251844785448],
                        [ 0.170951464116,  0.620589570741,  0.752027025817],
                        [ 0.644436340629,  0.594155331411,  0.751257280077],
                        [ 0.433383145067,  0.531364696585,  0.750299972471],
                        [ 0.913189794302,  0.558383047186,  0.752416881325],
                        [ 0.026231675955,  0.618784636072,  0.252271595444],
                        [ 0.53259454872 ,  0.532236145871,  0.252032046541],
                        [ 0.317481054934,  0.600601951946,  0.251033925492],
                        [ 0.789751223388,  0.601718597951,  0.251406360855],
                        [ 0.167083201027,  0.436060886381,  0.751589951708],
                        [ 0.66625444467 ,  0.408168011309,  0.750831076838],
                        [ 0.414455736909,  0.381036631298,  0.75073376285 ],
                        [ 0.918509988264,  0.406872002392,  0.75134336541 ],
                        [ 0.042358076647,  0.432009102577,  0.251795346387],
                        [ 0.542127066775,  0.379074826481,  0.251232229967],
                        [ 0.290954045248,  0.419398557609,  0.250754738309],
                        [ 0.791230540441,  0.417462836365,  0.250874646151]]
```

$O_{3/8}MoTe_{2-3/8}$-2

```
==============================
# Set up lattice
vector_a = [23.3663, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.918, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.44384]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Tellurium, Tellurium, Oxygen, Tellurium, Oxygen, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.083366353623,  0.543703218291,  0.75143722006 ],
                        [ 0.572574154334,  0.475002572489,  0.746692357665],
                        [ 0.35387561055 ,  0.497380235098,  0.746955273913],
                        [ 0.81856604186 ,  0.504346273805,  0.751306672562],
                        [ 0.218517396484,  0.531384551644,  0.249636579348],
                        [ 0.707607885705,  0.490957987081,  0.250078258142],
                        [ 0.464149151563,  0.470430035176,  0.246505534558],
                        [ 0.947407229669,  0.532812063993,  0.251538771131],
                        [ 0.178992832249,  0.628745226385,  0.749949437557],
                        [ 0.652465381092,  0.580707081049,  0.749603016951],
                        [ 0.436427550702,  0.526631398134,  0.744828277287],
                        [ 0.888190459373,  0.617402568468,  0.751572455331],
                        [ 0.032751118754,  0.633887745047,  0.251584974747],
                        [ 0.536064609564,  0.524490036643,  0.246095143188],
                        [ 0.323998332905,  0.600683332634,  0.247250414967],
                        [ 0.778949647322,  0.547557650621,  0.25153337226 ],
                        [ 0.166441825268,  0.444589355555,  0.749927279033],
                        [ 0.666900339532,  0.394739110326,  0.74942385631 ],
                        [ 0.413451623796,  0.376878974397,  0.746592623134],
                        [ 0.916834271671,  0.432533861429,  0.751605779935],
                        [ 0.041294016414,  0.449535550901,  0.251731293858],
                        [ 0.541795451654,  0.370318688994,  0.246860377066],
                        [ 0.290275967897,  0.420267439458,  0.247710831643],
                        [ 0.794907391931,  0.396929004308,  0.250970378544]]
```

$O_{3/8}MoTe_{2-3/8}$-3

```
==============================
# Set up lattice
vector_a = [23.4375, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9274, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.44484]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Tellurium, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.081032091545,  0.508846869287,  0.747577529469],
                        [ 0.567590741044,  0.491265035471,  0.745239213846],
                        [ 0.348170062926,  0.490259378989,  0.744989986736],
                        [ 0.831326533339,  0.532772991146,  0.747498262332],
                        [ 0.210725951628,  0.509651309454,  0.246260977878],
                        [ 0.696233838159,  0.522248919254,  0.245817723092],
                        [ 0.45959974698 ,  0.474636918435,  0.245101309408],
                        [ 0.97026856971 ,  0.519235836614,  0.248221259615],
                        [ 0.166241988677,  0.605541218642,  0.745875147048],
                        [ 0.635942558862,  0.605473436175,  0.745214508843],
                        [ 0.428017674865,  0.527493361516,  0.745039546964],
                        [ 0.928529803691,  0.617104488962,  0.747778460232],
                        [ 0.048602054025,  0.559983662274,  0.24732088475 ],
                        [ 0.527077006448,  0.535680146927,  0.244956312372],
                        [ 0.310545751703,  0.589870141264,  0.24457091825 ],
                        [ 0.780724186989,  0.622573476899,  0.246984524078],
                        [ 0.16599412932 ,  0.417265330833,  0.746862311199],
                        [ 0.666670732805,  0.421734110022,  0.746164151356],
                        [ 0.416531643561,  0.37628766214 ,  0.745273745343],
                        [ 0.915083985373,  0.433896187962,  0.748752930801],
                        [ 0.040648169787,  0.408624706041,  0.248337246553],
                        [ 0.544515631274,  0.383365191485,  0.24570871948 ],
                        [ 0.29091440129 ,  0.40677259627 ,  0.245388575309],
                        [ 0.790465345288,  0.438272133329,  0.247650487795]]
```

$O_{3/8}MoTe_{2-3/8}$-4

```
==============================
# Set up lattice
vector_a = [23.4701, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9297, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.44099]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Oxygen, Oxygen, Oxygen, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.085030372434,  0.532212651922,  0.748638610993],
                        [ 0.57647208236 ,  0.488232435114,  0.75162102098 ],
                        [ 0.332811170058,  0.496948304711,  0.750392224893],
                        [ 0.820906078967,  0.505362254173,  0.748890563757],
                        [ 0.223166626159,  0.512540242638,  0.249832060096],
                        [ 0.710300943225,  0.496582859719,  0.250246141107],
                        [ 0.466169305642,  0.491045959181,  0.251808211802],
                        [ 0.950218484753,  0.528139530027,  0.248653007368],
                        [ 0.184629922976,  0.612100981951,  0.749811631966],
                        [ 0.659442929501,  0.589595150831,  0.750791812107],
                        [ 0.422862106638,  0.589179315124,  0.751858015537],
                        [ 0.893822702651,  0.61512116952 ,  0.74863939508 ],
                        [ 0.037992745687,  0.624726450931,  0.248672115382],
                        [ 0.542509606858,  0.537780450794,  0.251060140502],
                        [ 0.302466774499,  0.549958164829,  0.249734742848],
                        [ 0.783006969532,  0.550463828032,  0.248684754849],
                        [ 0.165280530336,  0.429607150294,  0.749573270551],
                        [ 0.666497988205,  0.402386769992,  0.750599057806],
                        [ 0.415399037164,  0.401599838088,  0.751825143201],
                        [ 0.916415030025,  0.429336842964,  0.748545889153],
                        [ 0.040870967798,  0.43972887699 ,  0.248436688385],
                        [ 0.542208454584,  0.385192599967,  0.252084917919],
                        [ 0.290039494033,  0.398425415054,  0.250350584728],
                        [ 0.794014617389,  0.399010523542,  0.249309549992]]
```

$O_{3/8}MoTe_{2-3/8}$-5

```
==============================
# Set up lattice
vector_a = [23.5097, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8708, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.44327]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium,
            Tellurium, Oxygen, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.080781921849,  0.519561506666,  0.759397675218],
                        [ 0.573677054483,  0.50274672901 ,  0.758225951801],
                        [ 0.329702141521,  0.498540510336,  0.758422390744],
                        [ 0.841315325395,  0.514791256153,  0.758909529197],
                        [ 0.219776583965,  0.508592944404,  0.258698516795],
                        [ 0.702207419944,  0.51946530341 ,  0.258538025711],
                        [ 0.462956585973,  0.500013342279,  0.257665199788],
                        [ 0.952114421285,  0.510786866728,  0.25866266504 ],
                        [ 0.177096247343,  0.6057157404  ,  0.760321470375],
                        [ 0.649890896962,  0.60958435058 ,  0.760023853517],
                        [ 0.41608245363 ,  0.595798465876,  0.759216035203],
                        [ 0.917480785966,  0.559629415997,  0.759182228508],
                        [ 0.032185255821,  0.613018889275,  0.26102231719 ],
                        [ 0.537649247316,  0.54992930479 ,  0.259455940089],
                        [ 0.297333478681,  0.550233398408,  0.259784658266],
                        [ 0.795361729836,  0.610317529269,  0.260451709466],
                        [ 0.16553740787 ,  0.421835163894,  0.757191433704],
                        [ 0.66595404216 ,  0.421664913642,  0.756810495107],
                        [ 0.415801237714,  0.407533587558,  0.756082980077],
                        [ 0.91648107377 ,  0.407644470991,  0.757251539201],
                        [ 0.040833805093,  0.424151153602,  0.257719471079],
                        [ 0.542695682211,  0.397756926677,  0.256132420458],
                        [ 0.291026375106,  0.397845371626,  0.25664900156 ],
                        [ 0.790348082217,  0.425924425712,  0.257480673132]]
```

$O_{4/8}MoTe_{2-4/8}$

==========

```
# Set up lattice
vector_a = [22.85, 0.0, 0.0]*Angstrom
vector_b = [0.0, 20.1192, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.40097]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Tellurium, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.095223126273,  0.552945510031,  0.749131250957],
                        [ 0.574673305162,  0.465483935111,  0.748016039016],
                        [ 0.34716641983 ,  0.471460197004,  0.749331122295],
                        [ 0.814419974304,  0.543011139509,  0.748818291396],
                        [ 0.23658064736 ,  0.512076542674,  0.249796725946],
                        [ 0.683327821264,  0.498228935383,  0.248019353735],
                        [ 0.460553160492,  0.456276861081,  0.247725003567],
                        [ 0.95496836163 ,  0.561385220584,  0.248414777172],
                        [ 0.20724466956 ,  0.615981759538,  0.749719832284],
                        [ 0.636891118057,  0.536454050349,  0.747777222369],
                        [ 0.428261239011,  0.511606485004,  0.74764061985 ],
                        [ 0.897524543839,  0.647111069161,  0.748253059673],
                        [ 0.052701714711,  0.649000121916,  0.248799531539],
                        [ 0.534313418901,  0.512560723742,  0.248485809699],
                        [ 0.323406527969,  0.530964183571,  0.249406790201],
                        [ 0.745400714913,  0.618634651033,  0.248653165014],
                        [ 0.166611155568,  0.441065675117,  0.749923994114],
                        [ 0.671906132537,  0.388972629407,  0.747957392232],
                        [ 0.413426350242,  0.360276307147,  0.74804155835 ],
                        [ 0.915333158133,  0.466136864745,  0.748560856853],
                        [ 0.041947967237,  0.46692104091 ,  0.249278704377],
                        [ 0.544061240021,  0.360769329922,  0.24805016711 ],
                        [ 0.286289001306,  0.386017773161,  0.249904642063],
                        [ 0.790848041346,  0.441035001776,  0.249004319123]]
```

$O_{4/8}MoTe_{2-4/8}$-1

```
==============================
# Set up lattice
vector_a = [23.0568, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8796, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.39885]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Tellurium, Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.091056752339,  0.544917694562,  0.75000410546 ],
                        [ 0.566146573219,  0.482670889527,  0.748489693153],
                        [ 0.343705661786,  0.474314017444,  0.750374766815],
                        [ 0.818145385964,  0.52245043814 ,  0.750564717108],
                        [ 0.232768863543,  0.510048319955,  0.250206798772],
                        [ 0.705141440767,  0.508320201386,  0.249754069665],
                        [ 0.456812232211,  0.465582440739,  0.250552764015],
                        [ 0.951644787827,  0.546222474088,  0.249053939561],
                        [ 0.199798148681,  0.613645579204,  0.750339162206],
                        [ 0.643523349551,  0.59406907942 ,  0.749442670276],
                        [ 0.422188755452,  0.519167859505,  0.751249285999],
                        [ 0.893223587485,  0.633287799291,  0.749157874984],
                        [ 0.0454329144  ,  0.640119674262,  0.250113172954],
                        [ 0.525324387416,  0.528631608261,  0.248625123356],
                        [ 0.318005218864,  0.533400976109,  0.250610979887],
                        [ 0.776659754356,  0.566286261656,  0.252644741798],
                        [ 0.16599642983 ,  0.434945656628,  0.74995924202 ],
                        [ 0.666636225056,  0.41012516222 ,  0.749096329989],
                        [ 0.414157703469,  0.365388279665,  0.750756714971],
                        [ 0.916388297403,  0.447559156956,  0.748863351852],
                        [ 0.041628373379,  0.455295256022,  0.24980221029 ],
                        [ 0.543791611129,  0.37467397441 ,  0.248666559662],
                        [ 0.286822976234,  0.384959111212,  0.249948957168],
                        [ 0.79440880891 ,  0.414747393377,  0.249421515874]]
```

$O_{4/8}MoTe_{2-4/8}$-2

```
==============================
# Set up lattice
vector_a = [23.1183, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8742, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.3975]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Oxygen, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.086416668463,  0.531808140181,  0.746382589286],
                        [ 0.564011568772,  0.493486769983,  0.747515407799],
                        [ 0.341797586189,  0.47534265034 ,  0.749619525075],
                        [ 0.840506424687,  0.531912665737,  0.74543262766 ],
                        [ 0.229992171823,  0.506090746972,  0.248618384611],
                        [ 0.694960573442,  0.526523841014,  0.247571234155],
                        [ 0.454872559549,  0.471553811933,  0.250943007856],
                        [ 0.954051843178,  0.527294538042,  0.244016579223],
                        [ 0.192175149208,  0.607561991848,  0.74810451558 ],
                        [ 0.63296322789 ,  0.609710172069,  0.747434737887],
                        [ 0.418571195453,  0.523760357781,  0.750371439216],
                        [ 0.918043358572,  0.576977968746,  0.743643917501],
                        [ 0.039507818803,  0.627464272203,  0.245691898053],
                        [ 0.521283889136,  0.536664972723,  0.248035206911],
                        [ 0.313922636386,  0.533260322785,  0.249661462236],
                        [ 0.786800459125,  0.623334430268,  0.245530190154],
                        [ 0.166609471037,  0.427281445817,  0.748324174965],
                        [ 0.665769035095,  0.425528373802,  0.747804881057],
                        [ 0.415739103262,  0.369672916279,  0.750854675442],
                        [ 0.917059800293,  0.424475875959,  0.744421322196],
                        [ 0.042058474823,  0.438370741378,  0.246413996553],
                        [ 0.544308464873,  0.384178674659,  0.248470630782],
                        [ 0.28841650365 ,  0.383369251682,  0.249552713532],
                        [ 0.790582680731,  0.440749297591,  0.246263421621]]
```

$O_{4/8}MoTe_{2-4/8}$-3

```
==============================
# Set up lattice
vector_a = [23.0202, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8718, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.39811]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.088242990536,  0.510365690992,  0.752771368211],
                        [ 0.561061621512,  0.498779205845,  0.751592848051],
                        [ 0.339244199634,  0.46581007818 ,  0.752917231453],
                        [ 0.831897432848,  0.552170944068,  0.750823846056],
                        [ 0.225823578987,  0.488890421   ,  0.252274669486],
                        [ 0.692549327594,  0.53928899496 ,  0.25121514603 ],
                        [ 0.452654872991,  0.469417383483,  0.251690070337],
                        [ 0.976955210642,  0.532411977239,  0.251359217678],
                        [ 0.189055608573,  0.591755930261,  0.752391323113],
                        [ 0.626165105895,  0.618354688042,  0.751539919165],
                        [ 0.413970071373,  0.518943798522,  0.752500505892],
                        [ 0.935092537018,  0.631997520395,  0.751361545746],
                        [ 0.059575604648,  0.566980758112,  0.253595251923],
                        [ 0.516015481144,  0.539251240445,  0.251566360512],
                        [ 0.309503702361,  0.521879356157,  0.253788689409],
                        [ 0.778211089311,  0.641689127899,  0.251176654818],
                        [ 0.165373720639,  0.406645528374,  0.751645486915],
                        [ 0.666108192314,  0.43697930408 ,  0.750864209604],
                        [ 0.418438822868,  0.364929483908,  0.751442122633],
                        [ 0.915657046848,  0.450891939737,  0.75057257364 ],
                        [ 0.039543213136,  0.4149445744  ,  0.251741004592],
                        [ 0.546735313311,  0.388526042549,  0.251307758781],
                        [ 0.29005864529 ,  0.370296507511,  0.252230785213],
                        [ 0.790265490338,  0.457362912075,  0.250467388243]]
```

$O_{4/8}MoTe_{2-4/8}$-4

```
==============================
# Set up lattice
vector_a = [23.2121, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8804, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.40072]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Oxygen, Tellurium, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.07857847268 ,  0.523061154266,  0.749376159087],
                        [ 0.578723733605,  0.522027850067,  0.75122165625 ],
                        [ 0.335577902915,  0.49403081536 ,  0.751875887526],
                        [ 0.835571388013,  0.49353816918 ,  0.751722528993],
                        [ 0.222061424021,  0.511503610608,  0.2516721657  ],
                        [ 0.722131184289,  0.510671138216,  0.253003264223],
                        [ 0.446110514225,  0.504185791484,  0.249805244035],
                        [ 0.945814748072,  0.504348477251,  0.248576865115],
                        [ 0.177481930388,  0.608806254824,  0.751182559172],
                        [ 0.67755430599 ,  0.607927183002,  0.752910827069],
                        [ 0.406342201424,  0.551674063526,  0.748162678764],
                        [ 0.906002170709,  0.551805542719,  0.746558457887],
                        [ 0.02384521653 ,  0.612685321807,  0.24918003288 ],
                        [ 0.524302682428,  0.611884108789,  0.251033656334],
                        [ 0.303252904462,  0.547776706405,  0.254324349385],
                        [ 0.803188011482,  0.547281193108,  0.254920560402],
                        [ 0.16566278946 ,  0.426201569053,  0.751166770165],
                        [ 0.665830042672,  0.425292294707,  0.752694835693],
                        [ 0.417477854708,  0.398007687602,  0.750166343194],
                        [ 0.917728964847,  0.397706266458,  0.748931085485],
                        [ 0.041158555689,  0.426020966163,  0.249127787382],
                        [ 0.541202592199,  0.424970103485,  0.251018295891],
                        [ 0.29033727778 ,  0.396077947194,  0.251711543416],
                        [ 0.790546425503,  0.395309299178,  0.2523120528  ]]
```

$O_{4/8}MoTe_{2-4/8}$-5

```
==============================
# Set up lattice
vector_a = [23.1166, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9013, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.40001]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Tellurium, Oxygen,
            Oxygen, Tellurium, Oxygen, Tellurium, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.07251147445 ,  0.541036383132,  0.747076425743],
                        [ 0.576108778569,  0.488055666963,  0.746680075448],
                        [ 0.353680974678,  0.518676674774,  0.745766445152],
                        [ 0.830218723133,  0.486937335364,  0.750009374541],
                        [ 0.211641131657,  0.545448648953,  0.246399719813],
                        [ 0.715280897787,  0.491216284996,  0.250403905494],
                        [ 0.465824600661,  0.48962908481 ,  0.246313241496],
                        [ 0.940089320684,  0.508572434134,  0.245761365699],
                        [ 0.162289927015,  0.6378776902  ,  0.746131028575],
                        [ 0.665276459221,  0.586110700714,  0.749449634391],
                        [ 0.437539092418,  0.546945785242,  0.744970983127],
                        [ 0.896709701252,  0.551635873222,  0.745105471004],
                        [ 0.01057289041 ,  0.62435823035 ,  0.246782613144],
                        [ 0.541151768679,  0.539952636907,  0.246157438971],
                        [ 0.316894891381,  0.620228294565,  0.245496598412],
                        [ 0.79372752642 ,  0.536832417405,  0.254312582068],
                        [ 0.165968763504,  0.453413219632,  0.746795424667],
                        [ 0.666177937841,  0.399880003977,  0.74978590814 ],
                        [ 0.41290867454 ,  0.396930694122,  0.746649849046],
                        [ 0.919890843626,  0.399989025951,  0.74644181223 ],
                        [ 0.04137082668 ,  0.440659337526,  0.247396986525],
                        [ 0.540255659356,  0.385138369676,  0.246788444234],
                        [ 0.290571946884,  0.439737133292,  0.246178348587],
                        [ 0.793324314214,  0.384228293467,  0.250325396922]]
```

$O_{5/8}MoTe_{2-5/8}$

==========

```
# Set up lattice
vector_a = [22.5913, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9655, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.35539]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Tellurium, Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.08816604089 ,  0.570300049597,  0.751649857279],
                        [ 0.580402622911,  0.461381060003,  0.750824131587],
                        [ 0.34925779937 ,  0.486754361202,  0.752244273107],
                        [ 0.806236512   ,  0.516636596347,  0.75048200842 ],
                        [ 0.237892223369,  0.532841371027,  0.251532706669],
                        [ 0.696504147798,  0.479530853963,  0.250804410085],
                        [ 0.46403648503 ,  0.463714582336,  0.252446172638],
                        [ 0.942501321057,  0.561339573461,  0.25132977814 ],
                        [ 0.202184934183,  0.63624656561 ,  0.751750639407],
                        [ 0.652050858228,  0.523808722424,  0.750723636879],
                        [ 0.43361417664 ,  0.521781515773,  0.75605353377 ],
                        [ 0.872292695963,  0.638069881514,  0.751472723189],
                        [ 0.034574422552,  0.661400298224,  0.25185140851 ],
                        [ 0.542872894287,  0.513593573688,  0.250728389978],
                        [ 0.326044855097,  0.548622469927,  0.2513332262  ],
                        [ 0.757502731744,  0.553999246781,  0.250460571987],
                        [ 0.166306272672,  0.461564503954,  0.751382381681],
                        [ 0.671038043462,  0.372067763647,  0.750853822706],
                        [ 0.410718853995,  0.370480103829,  0.751655152853],
                        [ 0.915505912959,  0.4594047389  ,  0.750973140432],
                        [ 0.040868895682,  0.47893255486 ,  0.251438840897],
                        [ 0.541115724929,  0.359733228957,  0.250736437026],
                        [ 0.284720609029,  0.403377881015,  0.251338722195],
                        [ 0.797424815459,  0.406365728577,  0.250230442302]]
```

$O_{5/8}MoTe_{2-5/8}$-1

```
==============================
# Set up lattice
vector_a = [22.8433, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8069, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.3545]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Oxygen, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.083568601237,  0.553039679455,  0.749888609995],
                        [ 0.576817803259,  0.472862141771,  0.749879881685],
                        [ 0.347220273179,  0.485856831639,  0.749966888467],
                        [ 0.832337882886,  0.531207560531,  0.749554683466],
                        [ 0.235243059393,  0.526867021456,  0.250003589103],
                        [ 0.685640207974,  0.498645290681,  0.249651595661],
                        [ 0.461322980953,  0.468601595792,  0.249985662926],
                        [ 0.947866132201,  0.53877072453 ,  0.249428174128],
                        [ 0.193546038143,  0.628194087823,  0.749950924776],
                        [ 0.641856236968,  0.542395064101,  0.749663670819],
                        [ 0.428987537924,  0.525762189257,  0.749937573569],
                        [ 0.906359188234,  0.585470626147,  0.749495061694],
                        [ 0.030557545913,  0.645801691517,  0.249794872586],
                        [ 0.537150592814,  0.522556300263,  0.249818553452],
                        [ 0.321347868606,  0.546984262334,  0.250013928186],
                        [ 0.764950946363,  0.613385328323,  0.249521658705],
                        [ 0.167723128159,  0.450677900962,  0.749983984529],
                        [ 0.670558830999,  0.388848015958,  0.749671757324],
                        [ 0.412698721379,  0.371817457594,  0.75001150604 ],
                        [ 0.918818805886,  0.432297917703,  0.749457408766],
                        [ 0.042499911394,  0.457137741627,  0.249923631433],
                        [ 0.542180603201,  0.367972865559,  0.249951064473],
                        [ 0.286876732662,  0.398660913106,  0.249980783828],
                        [ 0.791308703999,  0.433063796541,  0.249595089796]]
```

$O_{5/8}MoTe_{2-5/8}$-2

```
==============================
# Set up lattice
vector_a = [22.8024, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.7991, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.35265]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.086350829108,  0.531349516494,  0.750651119092],
                        [ 0.574328176848,  0.479841782094,  0.750822431078],
                        [ 0.343564116247,  0.476871262105,  0.750678414989],
                        [ 0.81864742004 ,  0.551329820859,  0.750301231192],
                        [ 0.229349021477,  0.508731309522,  0.250573834927],
                        [ 0.684332128423,  0.511924848462,  0.250578588388],
                        [ 0.458874177993,  0.467634258361,  0.250785292671],
                        [ 0.972740385477,  0.550251074033,  0.250484964203],
                        [ 0.190594223581,  0.612289075083,  0.750359384342],
                        [ 0.637268499725,  0.551776597714,  0.750667991229],
                        [ 0.423403624902,  0.52219748381 ,  0.750760024653],
                        [ 0.917811370223,  0.643550015021,  0.750217946708],
                        [ 0.05451432212 ,  0.587771521449,  0.250615004415],
                        [ 0.532215886238,  0.526881238058,  0.250760441245],
                        [ 0.315245158215,  0.535815398848,  0.250567215494],
                        [ 0.752428069209,  0.632304066255,  0.250094245529],
                        [ 0.165752941662,  0.428362709629,  0.750738418599],
                        [ 0.67141063923 ,  0.401099420637,  0.750810122989],
                        [ 0.41537784118 ,  0.367696205139,  0.7509798958  ],
                        [ 0.915093258888,  0.463689383188,  0.750613212919],
                        [ 0.039970206742,  0.433993150918,  0.250821682114],
                        [ 0.544821644863,  0.372845401574,  0.251046030865],
                        [ 0.288162984922,  0.384962466187,  0.250818564556],
                        [ 0.79053442804 ,  0.449502709407,  0.250508266242]]
```

$O_{5/8}MoTe_{2-5/8}$-3

```
==============================
# Set up lattice
vector_a = [22.9563, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8483, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.35723]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Oxygen, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.069093672706,  0.521179611878,  0.750369064133],
                        [ 0.581963051655,  0.483420096353,  0.750756194932],
                        [ 0.353551137868,  0.520334336117,  0.750815735415],
                        [ 0.840076663276,  0.514154478903,  0.750589251364],
                        [ 0.204903060367,  0.539791508972,  0.251244150346],
                        [ 0.691723647343,  0.498343388919,  0.251090107999],
                        [ 0.467073001937,  0.489750008859,  0.251157674307],
                        [ 0.956936619744,  0.505174639224,  0.251693224926],
                        [ 0.149066779716,  0.629960337819,  0.751179766005],
                        [ 0.651984302087,  0.546318358832,  0.751004016319],
                        [ 0.437852911422,  0.548065677483,  0.750962247373],
                        [ 0.919760400554,  0.556874251396,  0.751253247972],
                        [ 0.027191605396,  0.567459095935,  0.250425851654],
                        [ 0.545566280114,  0.536543255524,  0.250738130242],
                        [ 0.310069749483,  0.619828370624,  0.250648424911],
                        [ 0.780745339893,  0.603449523887,  0.25018828546 ],
                        [ 0.166122141487,  0.442968071499,  0.751299561848],
                        [ 0.668398794525,  0.390629751651,  0.751436496086],
                        [ 0.413069498092,  0.397490868836,  0.75135426231 ],
                        [ 0.916766741731,  0.403765617023,  0.7522367708  ],
                        [ 0.043036661104,  0.413601549803,  0.250622765875],
                        [ 0.53991127221 ,  0.382341216898,  0.250690106632],
                        [ 0.290794234222,  0.439704459075,  0.25090730809 ],
                        [ 0.790971519884,  0.421817318493,  0.250624153525]]
```

$O_{5/8}MoTe_{2-5/8}$-4

```
==============================
# Set up lattice
vector_a = [22.9956, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8245, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.35355]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen,
            Tellurium, Oxygen, Tellurium, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.093558351688,  0.530776369687,  0.749524351617],
                        [ 0.579478409576,  0.48102095663 ,  0.749855010616],
                        [ 0.349920515458,  0.507196538695,  0.749992522512],
                        [ 0.835269190787,  0.525568709469,  0.749993277029],
                        [ 0.206653530899,  0.51981839137 ,  0.249994871962],
                        [ 0.68836362402 ,  0.501157811012,  0.249981980623],
                        [ 0.464525530146,  0.482888898325,  0.24933600142 ],
                        [ 0.948764780248,  0.526640624935,  0.249384880236],
                        [ 0.173301472753,  0.573740601968,  0.749841537065],
                        [ 0.647073398646,  0.547112392141,  0.750035382101],
                        [ 0.433634976889,  0.539791156045,  0.749457031361],
                        [ 0.910680239697,  0.57678557808 ,  0.749645707979],
                        [ 0.040660155179,  0.625685525823,  0.249425495285],
                        [ 0.54133383681 ,  0.532736780757,  0.24972468289 ],
                        [ 0.306026677643,  0.607671901787,  0.250348124279],
                        [ 0.771641198653,  0.611306258538,  0.250263409922],
                        [ 0.166390290774,  0.418971303727,  0.749885360276],
                        [ 0.669007996311,  0.392145032667,  0.749909952037],
                        [ 0.414311946746,  0.387611427487,  0.749228582366],
                        [ 0.917271223447,  0.421979833757,  0.749315372216],
                        [ 0.040993962562,  0.440728298068,  0.249364687473],
                        [ 0.54089510464 ,  0.378253439684,  0.249612961077],
                        [ 0.29102762656 ,  0.422915297731,  0.250005486561],
                        [ 0.790482142749,  0.429939267534,  0.249939333197]]
```

$O_{5/8}MoTe_{2-5/8}$-5

```
==============================
# Set up lattice
vector_a = [22.9586, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.8107, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.3526]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Oxygen, Tellurium, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.074047760841,  0.541256669778,  0.749950779857],
                        [ 0.5986584133  ,  0.505860034952,  0.749952883324],
                        [ 0.339633128244,  0.509161701763,  0.749937714323],
                        [ 0.828946190803,  0.485525795326,  0.749919852465],
                        [ 0.224529537521,  0.533697842467,  0.249952135331],
                        [ 0.713952673448,  0.483801805839,  0.249904270443],
                        [ 0.450617139095,  0.509111284657,  0.249939072698],
                        [ 0.939589821762,  0.508965412195,  0.249952498532],
                        [ 0.174783953649,  0.629590185542,  0.749980088678],
                        [ 0.681472440754,  0.540079385304,  0.749942449565],
                        [ 0.415029018354,  0.56196809005 ,  0.749940404526],
                        [ 0.89544980906 ,  0.552444913071,  0.749945787731],
                        [ 0.012936570299,  0.626786516895,  0.249972457594],
                        [ 0.548293216324,  0.602532805451,  0.249966367837],
                        [ 0.307576154957,  0.565896888087,  0.249951581498],
                        [ 0.789925776328,  0.536067417965,  0.249910857748],
                        [ 0.165942475609,  0.448655567596,  0.749930289519],
                        [ 0.665518107897,  0.3873714229  ,  0.749875503072],
                        [ 0.416063553339,  0.405310659392,  0.749926437894],
                        [ 0.920177052613,  0.399243766629,  0.749954201494],
                        [ 0.041279304717,  0.44129919911 ,  0.249925785587],
                        [ 0.541444262636,  0.41962835338 ,  0.249936605589],
                        [ 0.289120142302,  0.413823717924,  0.249920940524],
                        [ 0.792627227677,  0.381506158806,  0.249900774997]]
```

$O_{6/8}MoTe_{2-6/8}$

==========

```
# Set up lattice
vector_a = [22.4512, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9266, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.30839]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen,
            Tellurium, Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.113305122264,  0.558276594199,  0.750112233774],
                        [ 0.577974739788,  0.473763999669,  0.750507994487],
                        [ 0.34149820225 ,  0.479864411343,  0.750360766217],
                        [ 0.806251265258,  0.533392012419,  0.749821875848],
                        [ 0.225778276401,  0.508504387309,  0.250241500032],
                        [ 0.695492978591,  0.495817594002,  0.25017688206 ],
                        [ 0.459464796064,  0.46822084024 ,  0.250491048958],
                        [ 0.945874629059,  0.574441223591,  0.250183737227],
                        [ 0.201097968847,  0.572050001657,  0.750163823142],
                        [ 0.648911373442,  0.538905845985,  0.750418224715],
                        [ 0.424221779651,  0.523756140134,  0.750426510931],
                        [ 0.877130172745,  0.654479663027,  0.750046860142],
                        [ 0.060346520354,  0.654617511154,  0.249943522705],
                        [ 0.536711064892,  0.523506942117,  0.250540448523],
                        [ 0.312331778849,  0.539730638465,  0.250220457493],
                        [ 0.756947817546,  0.571122151605,  0.249476452765],
                        [ 0.158831926445,  0.427179020955,  0.750386954921],
                        [ 0.671943348124,  0.387356083091,  0.750565197928],
                        [ 0.412989665624,  0.369859194006,  0.750575158972],
                        [ 0.915796088786,  0.47408177601 ,  0.750331796153],
                        [ 0.041496587373,  0.484207164101,  0.250225557259],
                        [ 0.543237127047,  0.369814004991,  0.25059329285 ],
                        [ 0.283714661124,  0.389299447467,  0.2505165312  ],
                        [ 0.797356694602,  0.422457848385,  0.250291655539]]
```

$O_{6/8}MoTe_{2-6/8}$-1

```
==============================
# Set up lattice
vector_a = [20.422, 0.0, 0.0]*Angstrom
vector_b = [0.0, 20.9534, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.30107]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen,
            Tellurium, Oxygen, Tellurium, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.131622196576,  0.658031226917,  0.737535992743],
                        [ 0.595245941303,  0.43087665482 ,  0.740082231969],
                        [ 0.351620802784,  0.499642218182,  0.738379009605],
                        [ 0.83046216333 ,  0.513654060063,  0.737459925325],
                        [ 0.225934146098,  0.574268943175,  0.238997003996],
                        [ 0.719650538381,  0.454323325609,  0.237646571864],
                        [ 0.468983173282,  0.446150872885,  0.238911241382],
                        [ 0.913238815788,  0.600704215133,  0.236942069357],
                        [ 0.225123379432,  0.637012276875,  0.738933736103],
                        [ 0.668135936726,  0.494158641929,  0.737593743581],
                        [ 0.450250384583,  0.506033798828,  0.738362555561],
                        [ 0.85445820396 ,  0.608387802204,  0.737375230951],
                        [ 0.143924866123,  0.760683115949,  0.236539422142],
                        [ 0.558571326353,  0.483813698636,  0.239584047298],
                        [ 0.357379881458,  0.605533609312,  0.237892006875],
                        [ 0.770301229938,  0.535682782241,  0.237399313233],
                        [ 0.128578203946,  0.526241896381,  0.738958533848],
                        [ 0.699268797136,  0.349313296007,  0.739303979402],
                        [ 0.390850538983,  0.371721701496,  0.739141430217],
                        [ 0.965275821039,  0.50982542258 ,  0.737190233501],
                        [ 0.020735469699,  0.646502620212,  0.23716180418 ],
                        [ 0.54216730258 ,  0.337181572654,  0.2408384559  ],
                        [ 0.258405577917,  0.448347541052,  0.238563751422],
                        [ 0.844810452479,  0.40754063776 ,  0.237967591616]]
```

$O_{6/8}MoTe_{2-6/8}$-2

```
==============================
# Set up lattice
vector_a = [22.4525, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.9642, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.30886]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Tellurium, Oxygen, Oxygen,
            Oxygen, Oxygen, Oxygen, Tellurium, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.05573827869 ,  0.532762862384,  0.749520333793],
                        [ 0.591025649929,  0.478370868291,  0.749354396863],
                        [ 0.363300261793,  0.557286675281,  0.749122504385],
                        [ 0.827414883858,  0.472592975701,  0.749071558183],
                        [ 0.194564819226,  0.574289397096,  0.24948250651 ],
                        [ 0.709003873652,  0.466988191544,  0.249427603796],
                        [ 0.475558435444,  0.507002863243,  0.249457229474],
                        [ 0.944989628311,  0.49443674143 ,  0.249221304419],
                        [ 0.125782490098,  0.654054702836,  0.749603998197],
                        [ 0.673637724809,  0.522232165376,  0.749341721123],
                        [ 0.45091533854 ,  0.570458097344,  0.74955326562 ],
                        [ 0.89854153541 ,  0.537503526719,  0.749085259361],
                        [ 0.006357110986,  0.570141279532,  0.249504729342],
                        [ 0.562188391419,  0.538368921385,  0.249532730727],
                        [ 0.309420608064,  0.652960878242,  0.249104006272],
                        [ 0.786072069899,  0.522485767847,  0.249240402836],
                        [ 0.165344175407,  0.473861509807,  0.749427019701],
                        [ 0.662599309845,  0.368711248545,  0.749525589861],
                        [ 0.408239201868,  0.426161327637,  0.749274346546],
                        [ 0.921491648862,  0.386179253595,  0.748991509544],
                        [ 0.046960594673,  0.421978142628,  0.249576268658],
                        [ 0.533195877959,  0.387828524935,  0.249244324628],
                        [ 0.291016669666,  0.483668849437,  0.248995996301],
                        [ 0.792810100755,  0.36873374671 ,  0.248963618348]]
```

$O_{6/8}MoTe_{2-6/8}$-3

```
==============================
# Set up lattice
vector_a = [22.9016, 0.0, 0.0]*Angstrom
vector_b = [0.0, 19.7654, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.31756]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Tellurium,
            Oxygen, Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.093824529601,  0.541409955864,  0.74947751561 ],
                        [ 0.595981883779,  0.491985134005,  0.749410105279],
                        [ 0.319235545853,  0.532324324103,  0.749482430458],
                        [ 0.826042279924,  0.484123349194,  0.749390486359],
                        [ 0.210787701043,  0.524261563216,  0.24948280877 ],
                        [ 0.710635280582,  0.477693846601,  0.249355643205],
                        [ 0.483091190591,  0.53096045    ,  0.249410153606],
                        [ 0.93193440291 ,  0.511473704684,  0.249372992039],
                        [ 0.17375985578 ,  0.578804513676,  0.749498558047],
                        [ 0.676928386813,  0.534127270678,  0.749513669175],
                        [ 0.426692760721,  0.624573403395,  0.749452372796],
                        [ 0.889979317346,  0.556053948659,  0.749420983028],
                        [ 0.024945827432,  0.622971794346,  0.249550675906],
                        [ 0.567303638355,  0.55337570746 ,  0.249322308699],
                        [ 0.28310734781 ,  0.584300249334,  0.249547807936],
                        [ 0.785285592202,  0.53324784245 ,  0.249403310348],
                        [ 0.16505542583 ,  0.425237335533,  0.749420999701],
                        [ 0.663823841795,  0.379281767586,  0.749214520208],
                        [ 0.417351633944,  0.450270979934,  0.749404768751],
                        [ 0.920783591422,  0.40094841972 ,  0.749282774239],
                        [ 0.040501622244,  0.449284005026,  0.249404150464],
                        [ 0.537390409657,  0.403389142661,  0.249333635802],
                        [ 0.292922674348,  0.425406971892,  0.249382318069],
                        [ 0.792891160384,  0.377881882564,  0.24931272939 ]]
```

$O_{6/8}MoTe_{2-6/8}$-4

==========

```
# Set up lattice
vector_a = [22.9685491458,0, 0]*Angstrom
vector_b = [0, 19.7647654588, 0]*Angstrom
vector_c = [0, 0, 3.31913826156]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen,
            Tellurium, Tellurium, Oxygen, Oxygen, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.101170789587,  0.530947801992,  0.748975967171],
                        [ 0.601146030009,  0.531122013424,  0.749543671048],
                        [ 0.331095785518,  0.499243020843,  0.749486270524],
                        [ 0.831227983292,  0.499084371636,  0.748916946586],
                        [ 0.2158140414  ,  0.502652121538,  0.249221383397],
                        [ 0.715908772678,  0.502668851114,  0.249189084187],
                        [ 0.438056313592,  0.516993923194,  0.249455929186],
                        [ 0.938195699429,  0.516822215978,  0.248567440897],
                        [ 0.183342690209,  0.560996265534,  0.748770470193],
                        [ 0.683359190171,  0.561038205429,  0.749558149049],
                        [ 0.399195089404,  0.565573381131,  0.749531576682],
                        [ 0.899335133016,  0.565415863211,  0.748691694537],
                        [ 0.038700926487,  0.618894290487,  0.248844111106],
                        [ 0.538552604917,  0.619012176955,  0.249548623484],
                        [ 0.293287368336,  0.55143739834 ,  0.249428709534],
                        [ 0.793492337624,  0.551294073092,  0.248923740612],
                        [ 0.163918537674,  0.408766500785,  0.74934252785 ],
                        [ 0.663887237233,  0.408895767224,  0.749296710107],
                        [ 0.419478170962,  0.407894626406,  0.749559860357],
                        [ 0.91958353084 ,  0.407731743581,  0.748679822852],
                        [ 0.041507750488,  0.44443969634 ,  0.249194584544],
                        [ 0.541410508436,  0.444635247391,  0.249600651501],
                        [ 0.290869912493,  0.396365619904,  0.249509340777],
                        [ 0.790886095834,  0.39622450512 ,  0.249161481896]]
```

$O_{7/8}MoTe_{2-7/8}$

==========

```
# Set up lattice
vector_a = [20.2479, 0.0, 0.0]*Angstrom
vector_b = [0.0, 21.0054, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.2578]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen,
            Tellurium, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.149963096329,  0.64849529901 ,  0.7520456016  ],
                        [ 0.592453831101,  0.440467171244,  0.74944932179 ],
                        [ 0.341206079259,  0.483018159237,  0.744424258724],
                        [ 0.829320830642,  0.530505490951,  0.750963142659],
                        [ 0.233861743763,  0.551672276856,  0.250414304289],
                        [ 0.717701907155,  0.469907868631,  0.250271313173],
                        [ 0.463669142677,  0.445075749562,  0.248348880321],
                        [ 0.918721698678,  0.614295147767,  0.251893571102],
                        [ 0.241367744526,  0.615471268886,  0.75379260872 ],
                        [ 0.663325194606,  0.507120688843,  0.750065748122],
                        [ 0.437688389055,  0.504386576641,  0.746978832638],
                        [ 0.858008681517,  0.624019518247,  0.752714602289],
                        [ 0.176392356057,  0.748452161912,  0.252220939956],
                        [ 0.550731205713,  0.490709644128,  0.249525836714],
                        [ 0.332541233605,  0.547151336069,  0.243343818953],
                        [ 0.76752921347 ,  0.552548802943,  0.250623710452],
                        [ 0.129822839234,  0.51817260669 ,  0.75057011072 ],
                        [ 0.701536734001,  0.364022017656,  0.750091011315],
                        [ 0.39250582161 ,  0.362916724732,  0.747320324532],
                        [ 0.965046174884,  0.520866319653,  0.751634475506],
                        [ 0.035943789714,  0.650907564469,  0.251780551699],
                        [ 0.547081278286,  0.342864025594,  0.248990816085],
                        [ 0.249522975303,  0.422780970936,  0.245456544804],
                        [ 0.844240295065,  0.424443153413,  0.250578683686]]
```

OMoTe

```
================================
# Set up lattice
vector_a = [20.3336, 0.0, 0.0]*Angstrom
vector_b = [0.0, 30.0, 0.0]*Angstrom
vector_c = [0.0, 0.0, 3.21792]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Molybdenum,
            Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen,
            Oxygen, Oxygen, Oxygen, Oxygen, Tellurium, Tellurium, Tellurium,
            Tellurium, Tellurium, Tellurium, Tellurium, Tellurium]

# Define coordinates
fractional_coordinates=[[ 0.153902002923,  0.59335156512 ,  0.749954279187],
                        [ 0.594150120919,  0.442725037364,  0.74996175528 ],
                        [ 0.343766594775,  0.47366851116 ,  0.749986853625],
                        [ 0.830237612332,  0.507339155433,  0.750064859357],
                        [ 0.238683845325,  0.524295012978,  0.250048535359],
                        [ 0.719016993939,  0.464204190779,  0.249990023942],
                        [ 0.465906907361,  0.445606798251,  0.250042190513],
                        [ 0.918236547812,  0.567999793794,  0.250142960963],
                        [ 0.247502308106,  0.569353459721,  0.750061242929],
                        [ 0.664206705415,  0.490252624939,  0.750208291639],
                        [ 0.440180255529,  0.487213443888,  0.750156774988],
                        [ 0.856457278405,  0.57292075563 ,  0.750138540947],
                        [ 0.173008371078,  0.626166272919,  0.250078756483],
                        [ 0.552316670039,  0.477893664109,  0.250089396009],
                        [ 0.336542561039,  0.518928744331,  0.250081786836],
                        [ 0.768117677429,  0.522431396114,  0.250072706589],
                        [ 0.132986036464,  0.50349859943 ,  0.749966010202],
                        [ 0.703492640916,  0.389643025288,  0.749780569586],
                        [ 0.39300442961 ,  0.388634588102,  0.749822472696],
                        [ 0.96576284634 ,  0.502543828514,  0.749944688937],
                        [ 0.03423715366 ,  0.598982115466,  0.249966721187],
                        [ 0.548680782231,  0.373833727081,  0.249791708361],
                        [ 0.250302815765,  0.43318940576 ,  0.249825041701],
                        [ 0.845876477805,  0.432758088605,  0.249873002275]]
```