

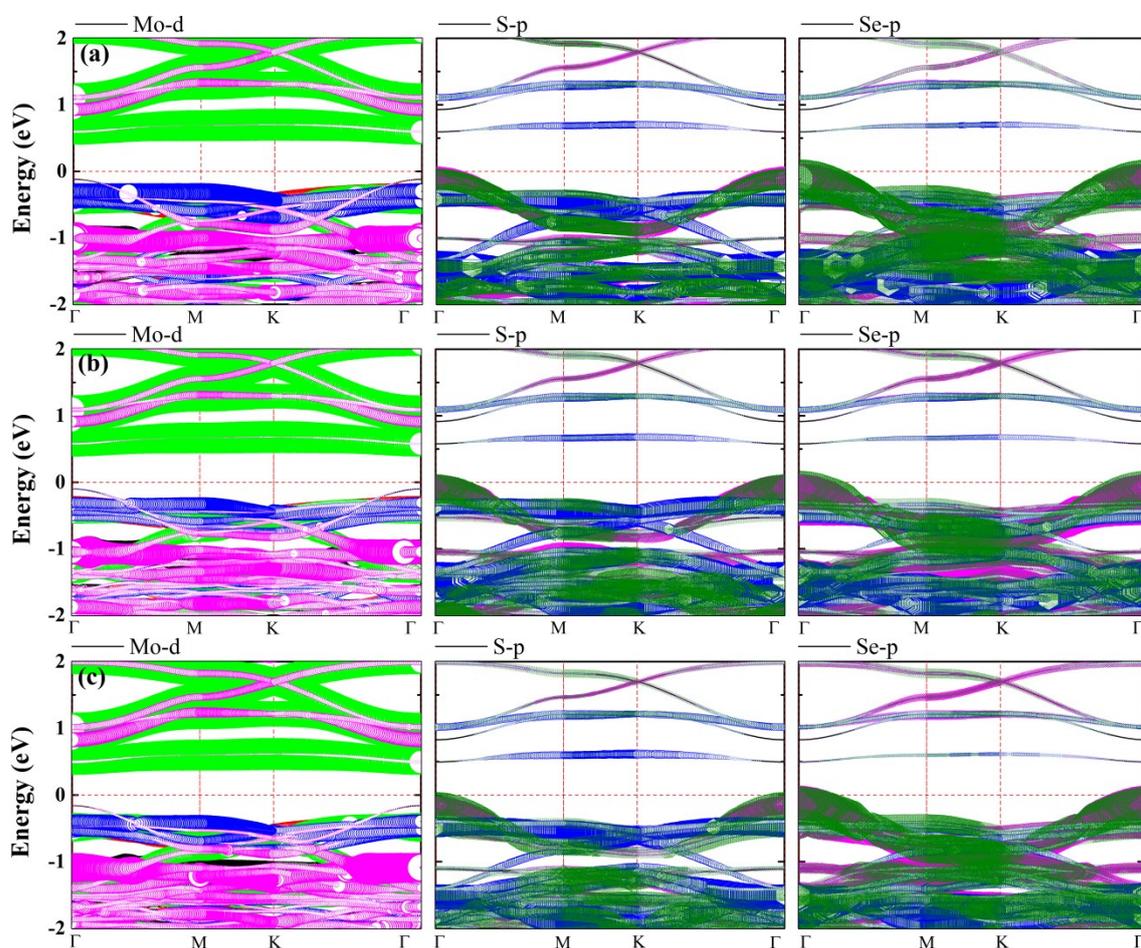
## First-principles investigation of novel Janus $\text{Mo}_8\text{S}_6\text{Se}_6$ monolayers as high-mobility semiconductors with bandgaps appropriate for low-power electronics

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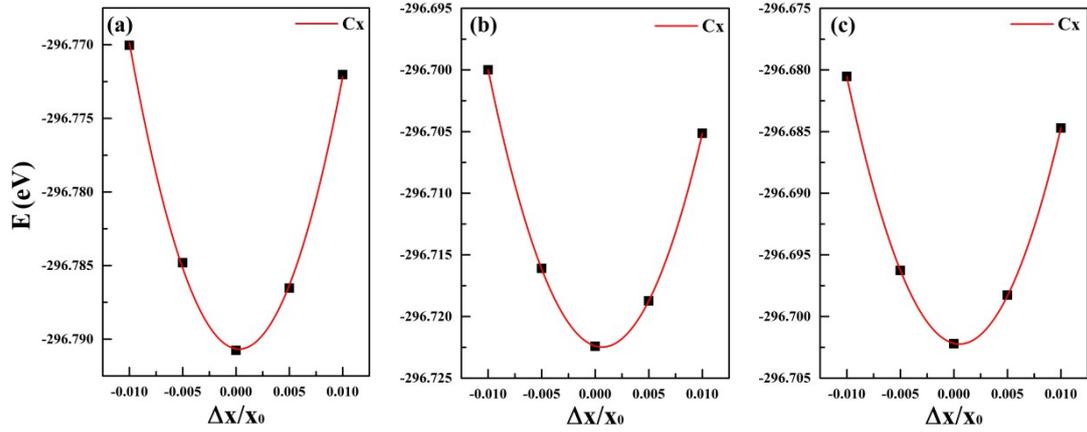
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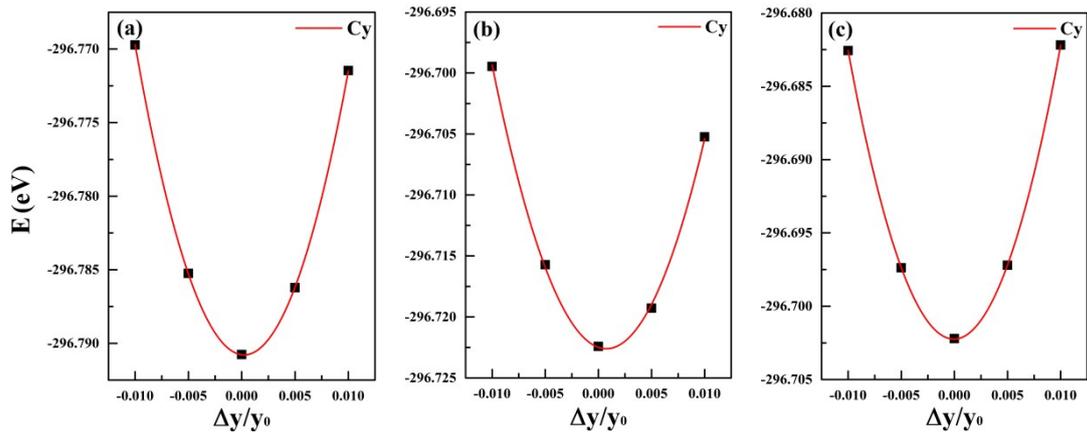
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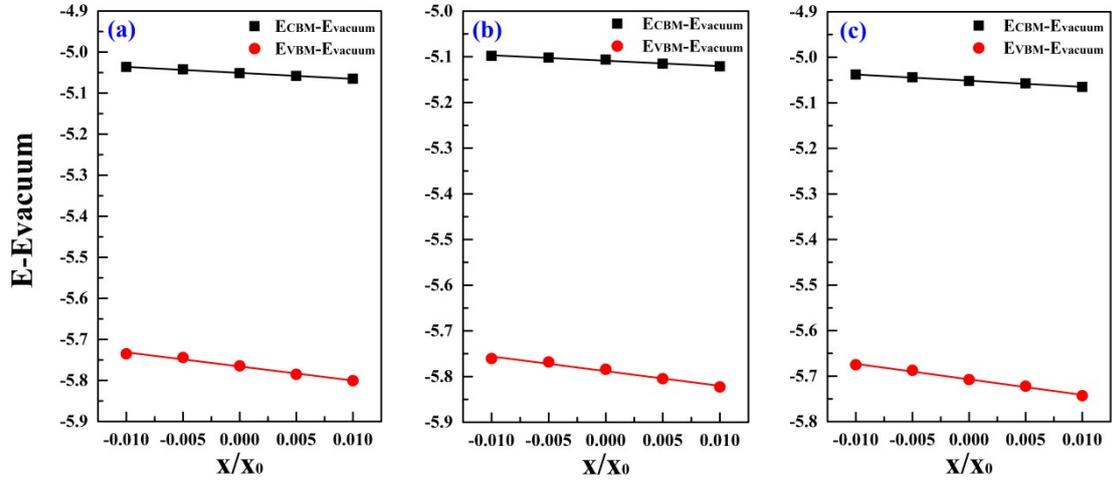
**Fig. S1.** The orbital-projected band structures of (a)  $P3m1$ , (b)  $Cmm2$ , and (c)  $C2/m$ - $\text{Mo}_8\text{S}_6\text{Se}_6$  monolayers. (The black, red, green, blue, and magenta colors represent the  $d_{xy}$ ,  $d_{yz}$ ,  $d_{z^2}$ ,  $d_{xz}$ , and  $d_{x^2-y^2}$  orbitals of the Mo atom, respectively, while the magenta, blue, and olive colors denote the  $p_y$ ,  $p_z$ , and  $p_x$  orbitals of the S and Se atoms, respectively.)



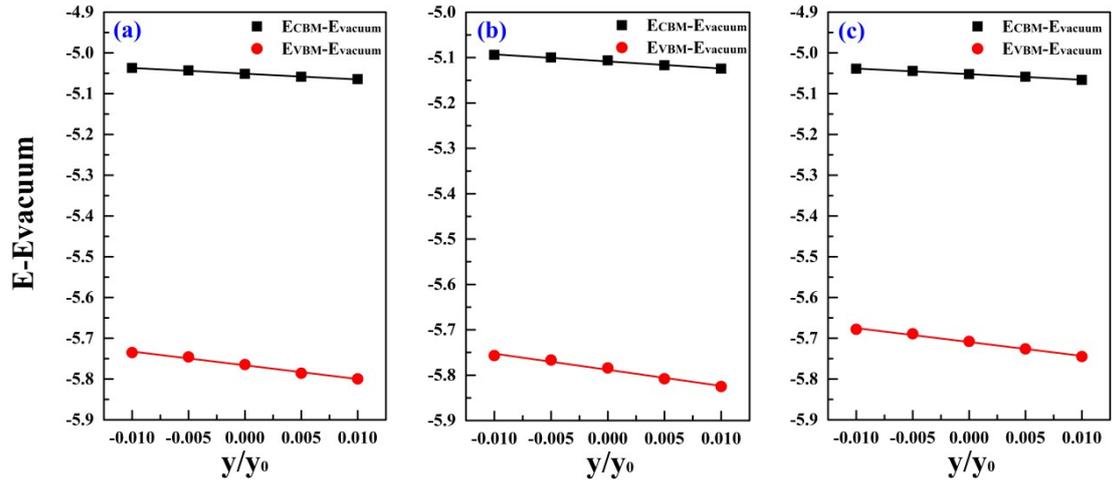
**Fig. S2.** The relationship between the total energy of (a) *P3m1*, (b) *Cmm2*, and (c) *C2/m*- $\text{Mo}_8\text{S}_6\text{Se}_6$  monolayers under uniaxial strain and the strain along the x direction, respectively. The in-plane stiffness  $C$  can be obtained after fitting the parabola.



**Fig. S3.** The relationship between the total energy of (a) *P3m1*, (b) *Cmm2*, and (c) *C2/m*- $\text{Mo}_8\text{S}_6\text{Se}_6$  monolayers under uniaxial strain and the strain along the y direction, respectively. The in-plane stiffness  $C$  can be obtained after fitting the parabola.



**Fig. S4.** The energy difference between the band energies of the CBMs and VBMs relative to the vacuum energy in (a)  $P3m1$ , (b)  $Cmm2$ , and (c)  $C2/m$ - $\text{Mo}_8\text{S}_6\text{Se}_6$  monolayers is illustrated as a function of lattice expansion along the x direction. The gradients of the black and red lines correspond to the DP constant in their respective directions for electrons and holes.



**Fig. S5.** The energy difference between the band energies of the CBMs and VBMs relative to the vacuum energy in (a)  $P3m1$ , (b)  $Cmm2$ , and (c)  $C2/m$ - $\text{Mo}_8\text{S}_6\text{Se}_6$  monolayers is illustrated as a function of lattice expansion along the y direction. The gradients of the black and red lines correspond to the DP constant in their respective directions for electrons and holes.

## POSCAR:

### *P3m1*-Mo<sub>8</sub>S<sub>6</sub>Se<sub>6</sub>

```
1.0000000000000000
  9.3353383559458365    0.0000000000000000    0.0000000000000000
 -4.6676578229740677    8.0846468138732561    0.0000000000000000
  0.0000000000000000    0.0000000000000000    20.0000000000000000
```

```
Mo   S   Se
  8   6   6
```

Selective dynamics

Direct

```
-0.0000006624379014  0.3799034867127682  0.4999999494027735  T  T  T
 0.6200945253748130  0.6200952578060032  0.5000000601537186  T  T  T
 0.3799121041638308  0.0000000067640988  0.5000000286840808  T  T  T
-0.0000006808641030  0.6200892663877386  0.4999999775485002  T  T  T
 0.3799090667704766  0.3799097139947508  0.5000000689289464  T  T  T
 0.6200977868813768 -0.0000001487297137  0.4999999927416772  T  T  T
 0.6666712555971197  0.3333323570514610  0.5029688172912797  T  T  T
 0.3333377041262574  0.6666661386080810  0.4970311627425294  T  T  T
 0.4402648010547585  0.2201340162668621  0.4213489772646905  T  T  T
 0.7798651816234861  0.2201325108758934  0.4213498336184742  T  T  T
 0.7798636924719418  0.5597337046693674  0.4213492493439644  T  T  T
 0.2201300789159694  0.4402665680249567  0.5786506707122806  T  T  T
 0.2201310985787504  0.7798668541916485  0.5786510784978945  T  T  T
 0.5597320258622587  0.7798675397887624  0.5786503392634463  T  T  T
 0.5725292140409525  0.7862669539968654  0.4101774076846060  T  T  T
 0.2137315415513606  0.7862663657588439  0.4101762041113262  T  T  T
 0.2137301829961769  0.4274689709620495  0.4101769504528224  T  T  T
 0.7862612989729764  0.5725312548224887  0.5898232454119443  T  T  T
 0.7862631021420885  0.2137337549159378  0.5898222955789059  T  T  T
 0.4274665781774128  0.2137353361311391  0.5898238705661540  T  T  T
```

### *Cmm2*-Mo<sub>8</sub>S<sub>6</sub>Se<sub>6</sub>

```
1.0000000000000000
  9.3320349114607328    0.0000000000000000    0.0000000000000000
 -4.6675104097727198    8.0811457292898581    0.0000000000000000
  0.0000000000000000    0.0000000000000000    20.0000000000000000
```

```
Mo   S   Se
  8   6   6
```

Selective dynamics

Direct

```
0.0000905807703382  0.3798387289339043  0.4977854401607639  T  T  T
 0.6202112030267248  0.6202079219099922  0.5010122850942120  T  T  T
 0.3798313910623200  0.0000875182449478  0.4977859490531255  T  T  T
```

-0.0000910077662167	0.6201594433906088	0.4977856914513226	T	T	T
0.3797870011584564	0.3797914568050040	0.5010122749636281	T	T	T
0.6201660258146772	-0.0000869577221990	0.4977857029831821	T	T	T
0.6666418286485123	0.3333704525321399	0.4998170791793370	T	T	T
0.3333565520216412	0.6666288145029475	0.4998169513171811	T	T	T
0.4352589735793453	0.2208364064080522	0.4199385180916991	T	T	T
0.7791710761242988	0.5647451252770770	0.4199396786346695	T	T	T
0.5647404007477913	0.7791640820342052	0.4199384435923431	T	T	T
0.2208290909603352	0.4352555540321496	0.4199393663738175	T	T	T
0.2163939655998588	0.7835960389939742	0.5776345422763982	T	T	T
0.7836051190432189	0.2164032781769394	0.5776342553725338	T	T	T
0.7820853148659722	0.2179146098211147	0.4090520213609996	T	T	T
0.2179133720657805	0.7820856985705948	0.4090522441483669	T	T	T
0.2127206991507775	0.4328395843306348	0.5885167820907184	T	T	T
0.5671578359671278	0.7872785331836830	0.5885180893200609	T	T	T
0.7872788287608342	0.5671610152684408	0.5885164895771665	T	T	T
0.4328416443982088	0.2127226043057917	0.5885183749584888	T	T	T

**C2/m-Mo<sub>8</sub>S<sub>6</sub>Se<sub>6</sub>**

1.0000000000000000

9.3355597212390631	0.0000000000000000	0.0000000000000000
-4.6577428895661654	8.0907508831611725	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Mo Se S  
8 6 6

**Selective dynamics**

**Direct**

0.0001241686659915	0.3798545817885711	0.5002678558113027	T	T	T
0.6200207672463575	0.6200164060524750	0.5000008811458915	T	T	T
0.3798496823915076	0.0001222852925675	0.4997321596971110	T	T	T
-0.0001237733431539	0.6201478001779128	0.4997320126196393	T	T	T
0.3799804893196960	0.3799845372940074	0.4999993457980444	T	T	T
0.6201511369061861	-0.0001218588114338	0.5002675942750545	T	T	T
0.6667674231244410	0.3332071951235247	0.4988468540963384	T	T	T
0.3332283632526862	0.6667938868689859	0.5011528649193765	T	T	T
0.4321741678409894	0.2159941718512656	0.4104785308589909	T	T	T
0.7839893948752162	0.5677862421256172	0.4104754983683572	T	T	T
0.2185405832806221	0.7814556314868883	0.4110485035551643	T	T	T
0.2160087144366714	0.4322134002859764	0.5895244220205318	T	T	T
0.5678244467327752	0.7840057069351490	0.5895221741727593	T	T	T
0.7814571971274813	0.2185433551920904	0.5889518900426181	T	T	T
0.7845317530033304	0.2154716991217051	0.4205721270950935	T	T	T
0.5636727746854461	0.7815514674743509	0.4209439208812575	T	T	T

0.2184605609525571	0.4363708513536956	0.4209387764247434	T	T	T
0.2154668228744344	0.7845276987835775	0.5794277574148360	T	T	T
0.7815388221909716	0.5636273585397701	0.5790613833704809	T	T	T
0.4363264004357938	0.2184474920633067	0.5790556274324234	T	T	T