

Supporting Information

As₂S₃, As₂Se₃ and As₂Te₃ nanosheets: Superstretchable semiconductors with anisotropic carrier mobilities and optical properties

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1. Atomic structures in VASP POSCAR format.

As₂S₃ Single-layer

```
1.0000000000000000
  4.4565478770785676    0.0000000000000000    0.0000000000000000
  0.0000000000000000    11.3586428131330397    0.0000000000000000
  0.0000000000000000    0.0000002190398780    16.0000000000000000
As    S
  4      6
Direct
  0.1470184054197524    0.9776839827368167    0.6887287834054856
  0.6470185841413943    0.4776834832616674    0.7790583578762966
  0.1469763350112658    0.2662003801634338    0.6887857330475007
  0.6469778898592778    0.7662009364405205    0.7790015304777591
  0.9866464694417696    0.9089773362034305    0.8151821001991848
  0.4866404976576784    0.4089780183359392    0.6526051852682671
  0.4866654382906487    0.8349020606950012    0.6525363747958466
  0.9866695313801641    0.3349025991376285    0.8152510745476576
  0.4455842341161372    0.1219276070633198    0.7472568477822522
  0.9455816968064539    0.6219274337906382    0.7205293878497953
```

As₂S₃ Double-layer

```
1.0000000000000000
  4.3783708174226312    0.0000000000000000    0.0000000000000000
  0.0000000000000000    11.4586199205554848    0.0000000000000000
  0.0000000000000000    0.0000000000000000    32.0000000000000000
As    S
  8     12
Direct
  0.1476807229525636    0.9764001531148351    0.0821023790869207
  0.8866680497627411    0.0238772665910248    0.2827966721130776
  0.3845476789411656    0.5206238787009527    0.2366695950008403
  0.6498024329920845    0.4796540133580149    0.1282295078658254
  0.1467759572848243    0.2626517593597238    0.0855045099745444
  0.8875738457144559    0.7376260487057881    0.2793945690254456
  0.3915113425880539    0.2377367875308832    0.2388101260614465
  0.6428382800197165    0.7625410205346216    0.1260890085718868
  0.0440406091334183    0.0980180727110716    0.2204024687257566
  0.9903087721601976    0.9022595044164765    0.1444966103075791
  0.4903251986279764    0.4035568312536605    0.0659180015128657
  0.5440247331297903    0.5967210188085651    0.2989811172537996
  0.4900123471912655    0.8351999193980839    0.0626270828955719
  0.5443371209495235    0.1650779411413145    0.3022720080377560
  0.0433574409834475    0.6631311655411537    0.2163932380246875
  0.9909910420252519    0.3371466214819690    0.1485058568753162
  0.5871515494438349    0.8820153259917826    0.2504388159414133
  0.4471965794790087    0.1182625660671708    0.1144602551252533
  0.9482540911220213    0.6192453168391492    0.0965388319792146
  0.0860949520725384    0.3810324912263557    0.2683602390874521
```

1.2 AS2Se3 Single-layer

```
1.0000000000000000
  4.4329380980850432    0.0000000000000000    0.0000000000000000
  0.0000000000000000    12.0962864784322601    0.0000000000000000
  0.0000000000000000    0.0000000000000000    16.0000000000000000
As   Se
  4     6
Direct
0.1391577113197329    0.9820766577777462    0.7094611954566901
0.6388662362776714    0.4821039964613121    0.7943627316320843
0.1380285587681058    0.2619229220143922    0.7104187158773172
0.6384230657526899    0.7619271393894564    0.7934272775622162
0.9870913661965659    0.9053635920966059    0.8422273659281956
0.4867017030485243    0.4053654239248701    0.6616115766589203
0.4874966120760078    0.8385578428978278    0.6605154279984546
0.9870802902607068    0.3385552440965114    0.8433304986732750
0.4632864370828500    0.1217573585943228    0.7768619366632663
0.9635019706516559    0.6217207437508208    0.7269983208620872
```

As2Se3 Double-layer

```
1.0000000000000000
  4.3601426900604530    0.0000000000000000    0.0000000000000000
  0.0000000000000000    12.1836960300425350    0.0000000000000000
  0.0000000000000000    0.0000000000000000    30.0000000000000000
As   Se
  8    12
Direct
0.1290778006839928    0.9833715911468249    0.0842022324832422
0.9081803132203292    0.0167657163496198    0.2990605508024734
0.4066191997568521    0.5126733100829902    0.2499000769787249
0.6306402455322430    0.4874645065007194    0.1333627531641222
0.1238445915157327    0.2633637581923829    0.0903481208382409
0.9134145824649467    0.7367740192181322    0.2929146667331913
0.4201497822435694    0.2376830360935972    0.2548118460142340
0.6171091202118224    0.7624547608624493    0.1284510096643395
0.0565120395877425    0.0985921407657860    0.2289730677670713
0.9807468077818502    0.9015453429689680    0.1542897282686516
0.4780413743397016    0.4048923182730638    0.0634930817049612
0.5592178900771164    0.5952454199642568    0.3197697654378980
0.4818282966266096    0.8422254200918825    0.0569453659559240
0.5554305023802470    0.1579124161194831    0.3263174471512134
0.0575561271098335    0.6560601433763223    0.2217837937451063
0.9797016087844457    0.3440776340341857    0.1614790278620407
0.5826787251213347    0.8789199206051984    0.2595453877073876
0.4545787294883667    0.1212179351517057    0.1237173998640377
0.9517384079984404    0.6219949765892182    0.0938867201642558
0.0855198546809182    0.3781428008212898    0.2893760333357500
```

1.3 As₂Te₃ Single-layer

```
1.0000000000000000
  4.4586902569312423    0.0000000000000000    0.0000000000000000
  0.0000000000000000    13.1148798657304209    0.0000000000000000
  0.0000000000000000    0.0000000000000000    16.0000000000000000
As    Te
  4      6
Direct
0.1236157189792877    0.9858096511681538    0.6945001095466310
0.6236253649356485    0.4858073993371050    0.7732886945177313
0.1236754961633295    0.2580628461431047    0.6944478802677878
0.6236556575417254    0.7580628167288381    0.7733367520809367
0.9927269230368125    0.8999795028050741    0.8364194578146922
0.4927573983522038    0.3999735791446213    0.6313692101721884
0.4927130572048100    0.8439005761353755    0.6314245877740845
0.9927175882574986    0.3438908626917723    0.8363623665739865
0.4801517226618088    0.1219475665441792    0.7726713461316166
0.9801402532005312    0.6219488813383904    0.6951149106828183
```

As₂Te₃ Double-layer

```
1.0000000000000000
  4.3911023379122733    0.0000000000000000    0.0000000000000000
  0.0000000000000000    13.1851312463480443    0.0000000000000000
  0.0000000000000000    0.0000000000000000    32.0000000000000000
As    Te
  8     12
Direct
0.1151653011780240    0.9892635289554192    0.0718186530081866
0.9339983631709075    0.0106535007461943    0.2872536110251431
0.4336164326067333    0.5051965916502326    0.2360555481191540
0.6155485924441280    0.4947210170604635    0.1230167795141739
0.0967919078861499    0.2660654309349866    0.0836020412872074
0.9523728946241050    0.7338520519631615    0.2754702624794589
0.4585572468914805    0.2358143343944263    0.2445340953978032
0.5906073069614735    0.7641031485037288    0.1145382560688617
0.0646752919648605    0.0981970756723882    0.2157250009287850
0.9844890854357757    0.9017201197188456    0.1433472869712134
0.4782063243940797    0.4059569825600278    0.0525161597865846
0.5709584910647933    0.5939605183544145    0.3065561757800808
0.4913627369292897    0.8484837489281887    0.0415547885851879
0.5578016075511414    0.1514338597825073    0.3175175270814776
0.0654214515354425    0.6477214999464991    0.2029214060864675
0.9837419382589587    0.3521959650107362    0.1561508976801989
0.5799519671367364    0.8762874024763363    0.2430955332601172
0.4692110693141061    0.1236301972639069    0.1159767625398800
0.9648484226824081    0.6245952937041608    0.0790756185371393
0.0843156079587004    0.3753222430921141    0.2799966296295295
```

2- AIMD results for the thermal stability.

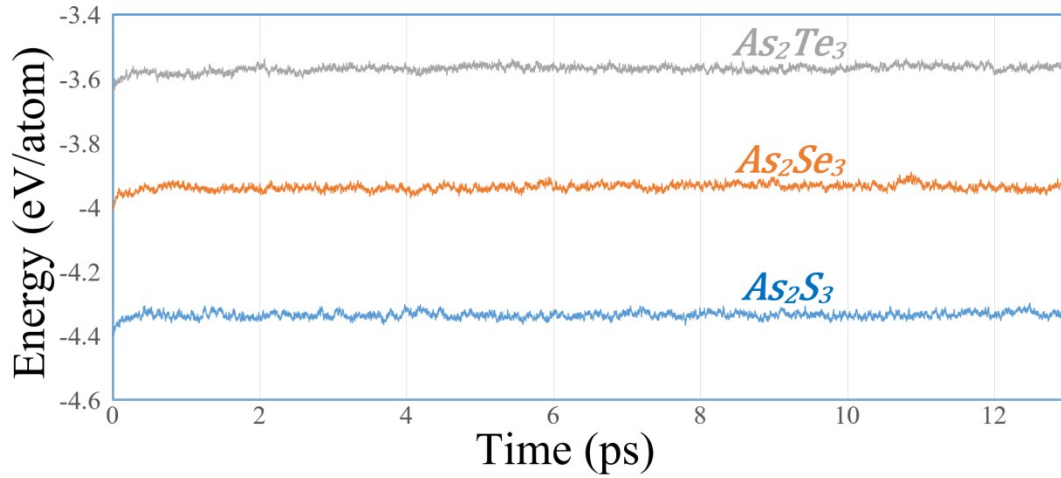


Fig. S1, Fluctuation of per atoms energy during the AIMD simulations at 500 K.

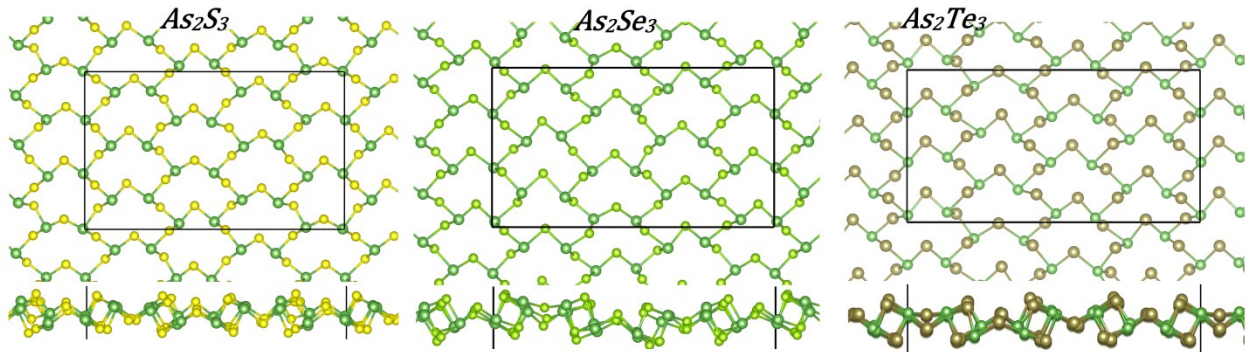


Fig. S2, Top and side views of studied monolayers after the AIMD simulations for 13 ps.

3- PBE results for the electronic band structures of monolayers with and without SOC.

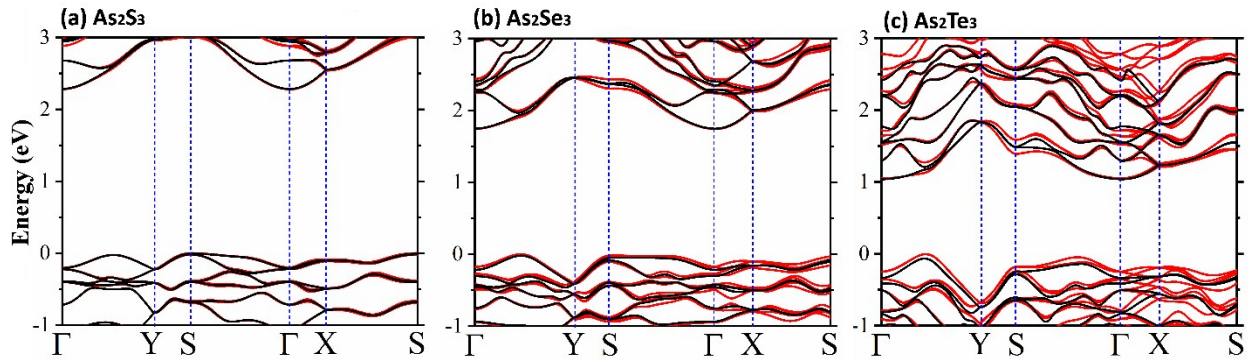


Fig. S3, PBE results for the electronic band structures of As_2S_3 , As_2Se_3 and As_2Te_3 monolayer with SOC (red lines) and without SOC (black lines).

4- HSE06 results for the electronic band structures of bulk systems.

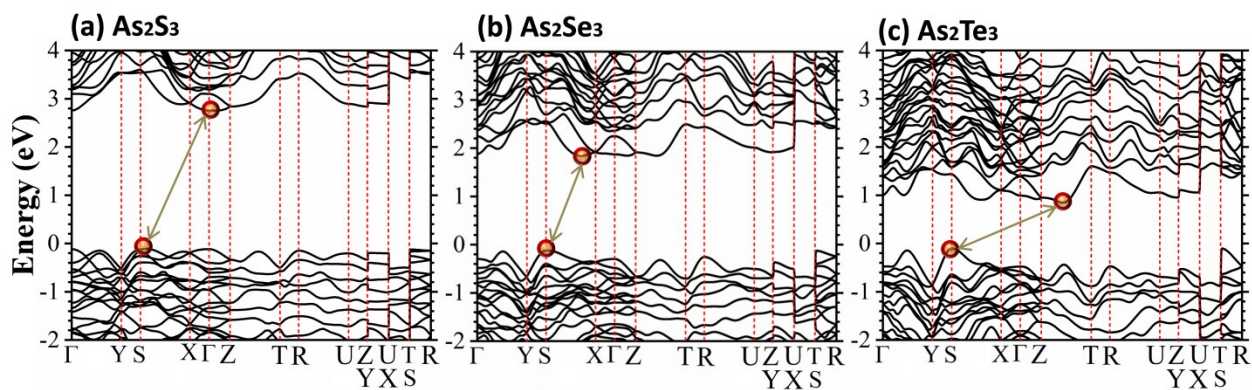


Fig. S4, HSE06 results for the electronic band structures of bulk As_2S_3 , As_2Se_3 and As_2Te_3 .

5- Charge density distributions of VBM and CBM states of As_2Se_3 and As_2Te_3 monolayers.

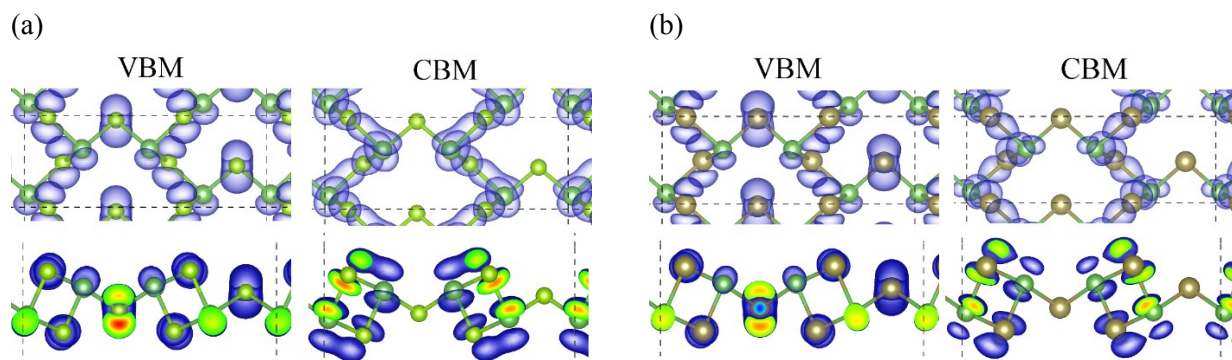


Fig. S5, HSE06 calculated charge density distributions of VBM and CBM states of (a) As_2Se_3 and (b) As_2Te_3 monolayers. The iso-surface value is set to $0.003 \text{ e}/\text{\AA}^3$.