

Electronic supplementary information for

Ultrahigh carrier mobility and multidirectional piezoelectricity in 2D Janus copper-containing chalcogenides monolayers

Mengbing Liu,^a Xingxu Meng,^a Yuli Yan,^a and Huabing Yin^{a,*}

^a*Institute for Computational Materials Science, Joint Center for Theoretical Physics, and Key Laboratory for High Efficiency Energy Conversion Science and Technology of Henan Province, School of Physics and Electronics, Henan University, Kaifeng 475004, China*

*E-mail: yhb@henu.edu.cn (Huabing Yin)

Crystal structure data

The following POSCAR files contain the structures of perfect CuP₂Se and Janus CuP₂Se_{0.5}S_{0.5} and CuP₂Te_{0.5}Se_{0.5} monolayers.

1. POSCAR of perfect CuP₂Se monolayer:

CuP₂Se

```
1.0000000000000000
 5.5899080641661039  0.0000000000000000  0.0000000000000000
 0.0000000000000000  6.4504556729256981  0.0000000000000000
 0.0000000000000000  0.0000000000000000  26.0000000000000000
```

```
Se Cu P
 4 4 8
```

Direct

```
0.0053013449331019  0.2462055813778292  0.2008942831013414
0.9946986672637621  0.7537943888961820  0.4364133974755831
0.5053013328432314  0.2537944186914416  0.4364133974755831
0.4946986672281000  0.7462055515825696  0.2008942831013414
0.1656701645168468  0.9273256967525825  0.2405119947159449
0.8343298205758742  0.0726743181642888  0.3967956668609816
0.6656701793528015  0.5726743031473589  0.3967956668609816
0.3343298205402121  0.4273256968372507  0.2405119947159449
0.3036626577344563  0.9802806909830863  0.3212780231499863
0.6963373125579793  0.0197193183919140  0.3160296764269361
0.8036626875490072  0.5197193090707941  0.3160296764269361
0.1963373572798091  0.4802806909138155  0.3212780231499863
0.6962833273027371  0.2840855898392007  0.2586693260274373
```

0.3037166727685872 0.7159144101454018 0.3786383355494891
0.1962833422456782 0.2159144100761310 0.3786383355494891
0.8037166728042564 0.7840855899084715 0.2586693260274373

2. POSCAR of Janus $\text{CuP}_2\text{Se}_{0.5}\text{S}_{0.5}$ monolayer:

CuP2Se0.5S0.5

1.0000000000000000
5.5201774925771447 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.4484397315325523 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000

Se S Cu P
2 2 4 8

Direct

0.0032390939102172 0.2447440849883762 0.2008578421818470
0.4967609205086418 0.7447440699972887 0.2008578421818470
0.9877479889342382 0.7566336368353674 0.4305489727930976
0.5122520110299789 0.2566336070237227 0.4305489727930976
0.1687832485293512 0.9285798605717872 0.2407310432342697
0.8373662713933498 0.0740788031514015 0.3981460947627085
0.6626337285708672 0.5740787881603140 0.3981460947627085
0.3312167365508856 0.4285798307601425 0.2407310432342697
0.3033255224261779 0.9801877973097888 0.3223885962261335
0.7005697305064587 0.0168982052449067 0.3165707818934962
0.7994302694577655 0.5168982237395952 0.3165707818934962
0.1966744775022633 0.4801878270284163 0.3223885962261335
0.6936131338040639 0.2809295901594453 0.2591939849455045
0.2905509219112119 0.7179480630380510 0.3807927081552620
0.2094490781961227 0.2179480481089797 0.3807927081552620
0.8063868661601532 0.7809295602857915 0.2591939849455045

3. POSCAR of Janus $\text{CuP}_2\text{Te}_{0.5}\text{Se}_{0.5}$ monolayer:

CuP2Te0.5Se0.5

1.0000000000000000
5.6852584372223260 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.4785399647393076 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000

Se Te Cu P
2 2 4 8

Direct

0.0082315020946169 0.2463833818084424 0.2010900565668621
0.4917685123242421 0.7463833668173550 0.2010900565668621
0.0032173935454480 0.7526643343490136 0.4434204055703006

0.4967826064187761 0.2526643045373689 0.4434204055703006
0.1613242035012163 0.9248272211390471 0.2401435285607789
0.8301073622443980 0.0709981331064640 0.3955477886667964
0.6698926377198191 0.5709981181153765 0.3955477886667964
0.3386757815790205 0.4248271913273953 0.2401435285607789
0.3037432092183394 0.9803927279114646 0.3198042698921100
0.6903079395094309 0.0231340808031604 0.3152946338929752
0.8096920604547932 0.5231340992978559 0.3152946338929752
0.1962567907101018 0.4803927576300921 0.3198042698921100
0.7001634411820419 0.2876801272538643 0.2581210797482925
0.3181992451306854 0.7139200349276749 0.3758082612941891
0.1818007549766492 0.2139200199986035 0.3758082612941891
0.7998365587821752 0.7876800973802034 0.2581210797482925