# Supplementary Material:

## Two-dimensional Janus $\alpha$-$Au_2XY$ ($X, Y$ = S/Se/Te) semiconductors with favourable band-gap and high carrier mobility by first-principles investigations

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**Table S1**. Atomic positions of Janus $\alpha$-$Au_2XY$ ($X/Y$ = S, Se,Te).

| | | $x$ | $y$ | $z$ |
|---|---|---|---|---|
| Janus $\alpha$-$Au_2SSe$ | Au1 | 0.5 | 0.507408166449272 | 0.358390690580377 |
| | Au2 | 0.0 | 0.99322295285337 | 0.357643929463856 |
| | S | 0.5 | 0.82620184992071 | 0.296451043606626 |
| | Se | 0.5 | 0.174167067776642 | 0.424514372349141 |
| Janus $\alpha$-$Au_2STe$ | Au1 | 0.5 | 0.518227356133014 | 0.358340755443204 |
| | Au2 | 0.0 | 0.982610295119442 | 0.355595155112203 |
| | S | 0.5 | 0.826650727226904 | 0.291043796096068 |
| | Te | 0.5 | 0.173511658520631 | 0.432020329348523 |
| Janus $\alpha$-$Au_2SeTe$ | Au1 | 0.5 | 0.511598232065798 | 0.359339053898884 |
| | Au2 | 0.0 | 0.989195404514621 | 0.357223150877916 |
| | Se | 0.5 | 0.829519690693376 | 0.284646317122251 |
| | Te | 0.5 | 0.1706867097262 | 0.435791514100957 |

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