Spin-orbit splitting and valence band anisotropy in Janus-like monolayers of rhenium dichalcogenides

Surani M. Gunasekera
Nourdine Zibouche, Daniel Wolverson, Marcin Mucha-Kruczynski
Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom.
smg28@bath.ac.uk

Monolayers of transition metal dichalcogenides (TMDs) consist of a layer of transition metal sandwiched between two layers of chalcogens. Interestingly, because of electronic similarities between different chalcogens, TMDs can also be engineered within a single layer, for example by swapping one plane of chalcogens from sulphur to selenium, resulting in so-called Janus layers (from the name of an ancient Roman god with two faces) which could be useful for potential applications in sensors, actuators, and novel electromechanical devices [1]. However, in a "regular" TMD like MoS_2, all chalcogens within one plane are related by C_3 symmetry and/or translation and hence are chemically equivalent. In contrast, in the rhenium dichalcogenides ReS_2 and $ReSe_2$, a lattice distortion lowers the symmetry of the crystal, leaving inversion as the only symmetry of the crystal and introducing in-plane anisotropy [2]. As a result, it might be possible to produce Janus-like layers in which only selected chalcogen sites in every unit cell are exchanged instead of a whole plane [3], providing a new degree of flexibility in material design. Here, we determine formation energies of all the possible ReS/Se Janus-like layers with substitutions in the top plane in order to determine the most stable configurations. We then study the changes in the electronic band structure introduced through the sulphur-selenium substitutions, including the appearance of spin-orbit splitting as a consequence of inversion symmetry-breaking.

References

[1] R. Li et al., Small, vol. 14 (2018), p. 1802091.
[2] D. Wolverson et al., ACS Nano, vol. 8 (2014), pp. 11154-11164.
[3] L. S. Hart, et al., npj 2D Materials and Applications 1.1 (2017): pp. 1-9.

Figures

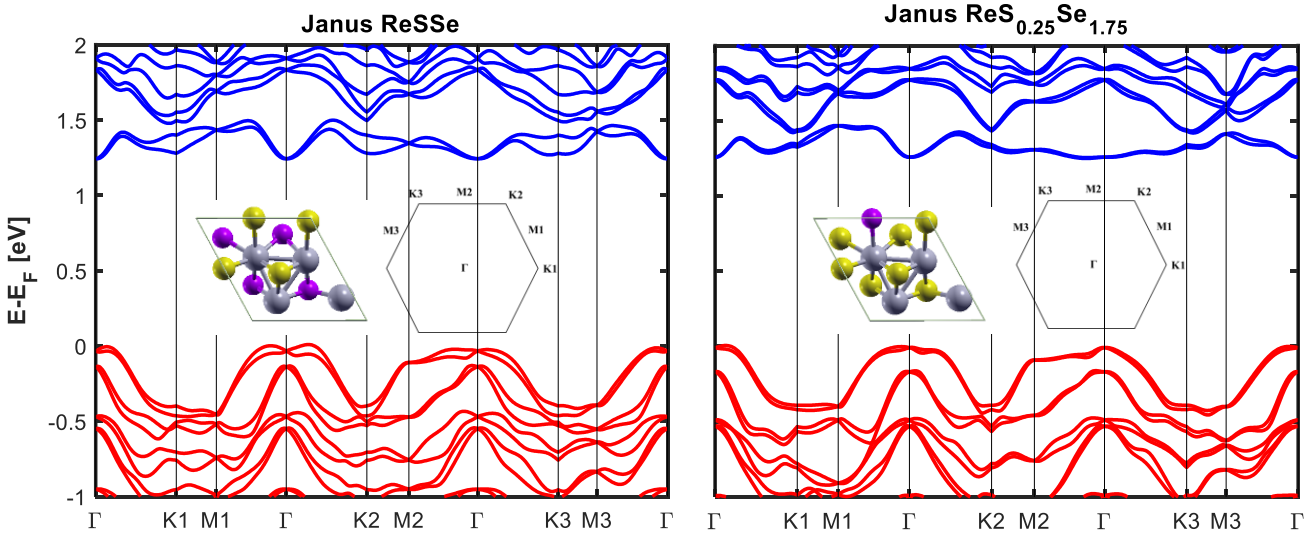

Figure 1: Left: Band structure plot for Janus ReSSe along special symmetry points, as marked in the figure of the Brillouin zone in the inset. Right: Band structure plot for Janus $ReS_{0.25}Se_{1.75}$ along special symmetry points, as marked in the inset. The figure in the inset of the graphs show the unit cell of the Janus monolayer, with Re in grey, S in purple and Se in yellow.