Electronic band structure of rhenium dichalcogenides and Janus monolayers

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Abstract

We study the electronic band structures of ReS_2 and $ReSe_2$ in the bulk and monolayer forms. These materials are layered transition metal dichalcogenides with only one symmetry operation – inversion, which is preserved even in monolayers. A lattice distortion that shifts the metal ions away from their positions in the centres of octahedrons formed by the chalcogen atoms leads to the formation of characteristic in-plane rhenium 'chains' [1][2]. For the bulk, we perform density functional theory (DFT) calculations across the full Brillouin zones rather than only the high-symmetry directions and show that both ReS_2 and $ReSe_2$ are indirect gap semiconductors [3]. We then contrast our ab initio results with angle-resolved photoemission spectroscopy (ARPES) data for monolayer, bilayer and bulk $ReSe_2$. We show that the highest valence band becomes flatter in the monolayer, indicating weak coupling between the Re chains and implying quasi 1D behaviour. Finally, we calculate the band structure of Janus monolayer ReSSe and find it to resemble more that of $ReSe_2$ than ReS_2.

References

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2. D. Wolverson, S. Crampin, A. S. Kazemi, A. Ilie and S. J. Bending, ACS Nano 2014, vol. 8, pp. 11154-11164.
3. S.M. Gunasekera, D. Wolverson, L.S. Hart, M. Mucha-Kruczynski, Journal of Elec Materi (2018).

Figures

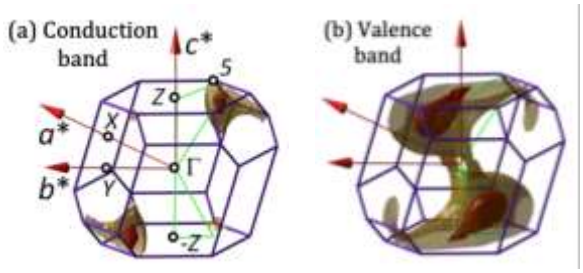

Figure 1: Bulk ReS_2: a) contours in the conduction band (CB) at energies of 70 meV (yellow) and 20 meV (red) above the CB minimum. b) Contours in the valence band (VB) at energies of 310 meV (yellow) and 70 meV (red) below the VB maximum. The VB maximum and CB minimum are not located in the same region, indicating an indirect band gap.

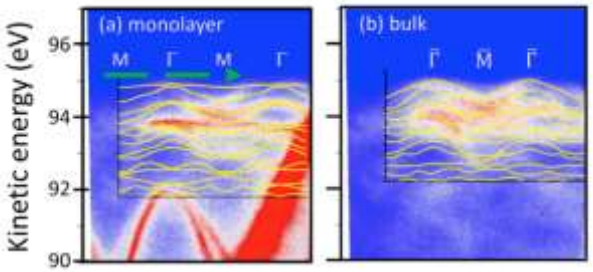

Figure 2: ARPES results of monolayer (a) and bulk (b) $ReSe_2$ in the direction Γ-M, with DFT results superimposed in yellow. Monolayer $ReSe_2$ has a very flat band at the top of the valence region, with the same band having significant curvature in bulk form.

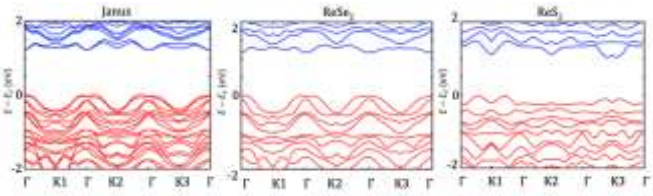

Figure 3: Band structures of Janus monolayer ReSSe (left), monolayer $ReSe_2$ (middle) and monolayer ReS_2 (right) along the paths Γ-K. It can be seen that the band structure of the Janus monolayer is much more similar to that of $ReSe_2$ than ReS_2.