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