Electronic band structure of rhenium dichalcogenides

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Abstract

The band structures of bulk transition metal dichalcogenides ReS_2 and $ReSe_2$ are presented, showing the complicated nature of the interband transitions in these materials, with several close-lying band gaps. Three-dimensional plots of constant energy surfaces in the Brillouin zone at energies near the band extrema are used to show that the valence band maximum and conduction band minimum are not located at any special high symmetry points. We show that, at the level of approximation of our calculations, both materials are indirect gap materials and that one must be careful to consider the whole Brillouin zone volume in addressing this question.

References

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Figures

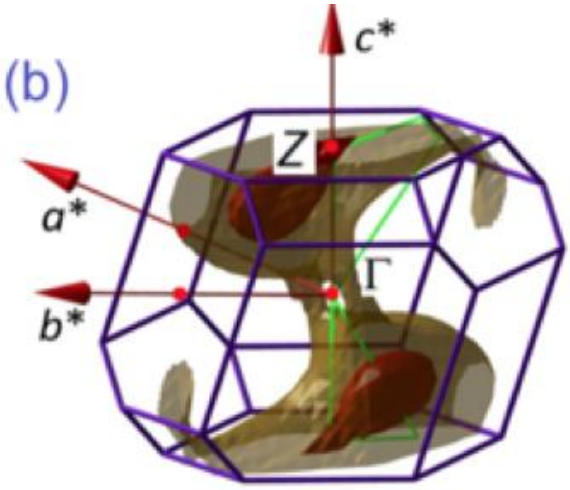

Figure 1: ReS_2: Contours in the valence band (VB) at energies of 310 meV (yellow) and 70 meV (red) below the VB maximum.

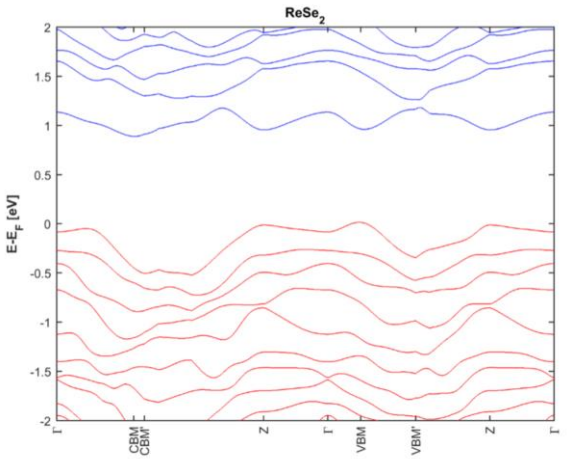

Figure 2: Conduction and valence band edges for $ReSe_2$ for a path around the Brillouin zone passing through the Γ and Z points and the band extrema (CBM and VBM). By passing a straight line through the CBM (VBM) and Γ point and continuing along this line to the BZ boundary, the CBM' (VBM') is found.