Quasiparticle Electronic Structure and Phonon-Driven Optical Properties of ZrS_3 : First-Principles Study

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Unlike two-dimensional materials such as graphene and transition metal dichalcogenides, transition metal trichalcogenides (MX_3) features as a quasi–one-dimensional chain-like structure that offers additional opportunities for tuning electronic and optoelectronic properties. In this study, we explore the electronic, optical, and vibrational characteristics of from bulk to monolaye $ZrSe_3$ using first-principles methods. The phonon dispersion relations revealed the dynamical stability of the systems. The electronic structure is first studied within the local density approximation, yielding indirect band gaps of 0.9889 eV for the bulk and 0.9674 eV for the monolayer. These results are further refined using the G_0W_0 approach. Optical properties are further analysed by solving the Bethe–Salpeter equation (BSE), allowing us to capture excitonic effects. The inherent structural anisotropy leads to direction-dependent electrical and optical responses. In addition, phonon contributions are included to account for lattice effects in the optical behaviour. These findings provide a good understanding of ZrS_3 and underline its potential for anisotropic electronic and optoelectronic applications in nano devices.

References

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Figures

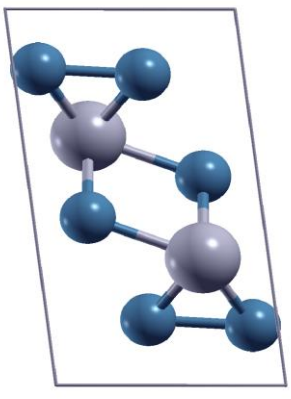

Figure 1: Crystal structure of ZrS_3

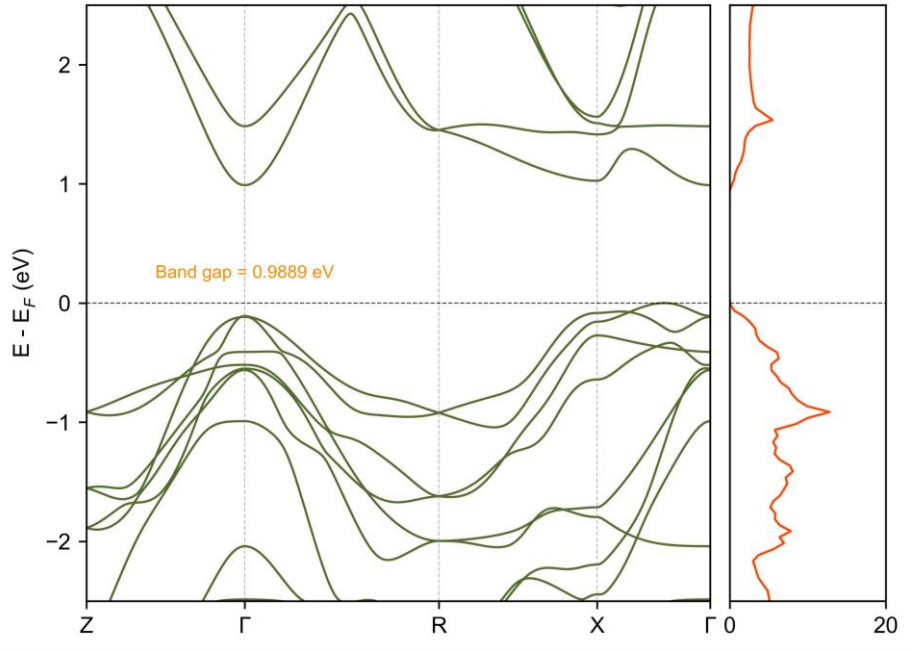

Figure 2: Bandstructure and total density of states (TDOS) of ZrS_3