Electronic and Optical Properties of Bilayer $PtSe_2$: Twist Angle and Pressure Dependence

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Abstract. Monolayer $PtSe_2$ is a transition metal dichalcogenide semiconductor with an indirect band gap and a 1T-type crystal structure. In addition to its promising electrical and optical properties, $PtSe_2$ offers excellent air stability, high room-temperature carrier mobility, and tunable band gap controlled by the number of layers. These features make $PtSe_2$ a highly promising material for applications in field-effect transistors, photodetectors, and sensors.

Using first-principles calculations based on density functional theory, we investigate the dependence of the electronic and optical properties of bilayer $PtSe_2$ on the twist angle. By analyzing the electronic structure and the imaginary part of the dielectric tensor, we find that the most significant changes in the dielectric function are observed between twist angles of 0° and 60°, while for angles between 13° and 32°, the optical properties remain relatively unchanged.

We also explore the impact of vertical strain on the system. Our numerical results show that an additional peak occurs at a photon energy of 1 eV due to gap reduction in the experimentally accessible strain values. Furthermore, for vertical stresses above 2.4 GPa, the bilayers with 0° and 60° twist angles undergo a transition to a metallic state. To refine the band gap prediction, we performed additional calculations using hybrid functionals. Compared to the Perdew-Burke-Ernzerhof (PBE) functional, the hybrid functional approach yields larger band gap values and higher photon absorption energies.

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