Electronic and optical properties of twisted $PtSe_2$

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Monolayer PtSe2 is a transition metal dichalcogenide semiconductor with an indirect gap and 1T-type crystal structure [1]. Besides promising electrical and optical properties, PtSe2 exhibits good air stability with high room-temperature carrier mobility and excellent tunability of the band gap by controlling the number of layers [2]. All of this makes PtSe2 a very promising material for field-effect transistor technology, photodetectors or sensors [3]. Using first principle calculations based on the density functional theory, we study the twist- angle dependence of electronic and optical properties of bilayer PtSe2. By examination of the electronic structure and imaginary part of the dielectric tensor, we find that the most significant changes in the dielectric function are observed between 0° and 60° twist angle, while for twist angles between 13° and 32°, optical properties do not differ much. We also study the effects of vertical strain on the electronic and optical properties. Our numerical results show that the additional absorption peak occurs at a photon energy of 1eV due to gap reduction in the experimentally accessible strain values [4]. For strains above 2.4GPa, the systems become metallic in the case of 0° and 60° twist angles. To improve the band gap size, we also performed calculations with hybrids functional. The values of band gap sizes and energy of photon absorption increase compared to the Perdew-Burke-Ernzerhof functional.

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[1] Wang et al. , *Nano Letters*, 15, 6, 4013-4018 (2015).
[2] Ciarrocchi et al. , *Nature Communications*, 9(1), 1–6 (2018).
[3] Zhao et al. Advanced Materials, 29(5) (2017).
[4] Fülöp et al. , *Npj 2D Materials and Applications*, 5(1), 1–6. (2021).