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Tuning the electronic properties and interfacial interactions of WS2/ZrO2(001) heterostructures by an external electric field, interlayer coupling and monolayer to few–layer of WS2 sheets

Understanding the connection between interfacial interactions and electronic properties are vital for the fabrication of ZrO2–based optoelectronic and nanoelectronics materials with desirable properties. In this study, the interfacial interactions, optical and electronic properties of WS2/ZrO2 heterostructures in the presence of an external electric field, interlayer coupling and monolayer to few–layer WS2 sheets are investigated for the first time using a first–principle calculations. All calculations were performed using the Cambridge Serial Total Energy Package (CASTEP) code [1] implemented in Materials Studio 2016 [2] with the plane-wave ultrasoft pseudopotentials method [3] and Perdew-Burke-Ernzerhof (PBE) functional for the exchange and correlation contribution [4]. All the simulations were done using the resources provided by the Centre for High Performance Computing (CHPC), Rosebank, Cape Town [5]. The charge density distribution and Mulliken population charge analysis reveal that the charge carriers can effectively separate in the layered WS2/ZrO2 interface. The optical absorption spectra and band shape of these hybrid heterostructures are similar, with their bandgap decreases, as well as their charge transfer and redshift of the absorption edge increase upon increasing the number of WS2 sheets. Moreover, by varying the interlayer coupling or by applying a suitable external electric field with different strengths, the cohesion energy, work function and bandgap energy of WS2/ZrO2 heterostructure can be effectively tuned. These theoretical results are expected to offer useful insights into the design of future optoelectronic and nanoelectronic devices based on two–dimensional van der Waals heterostructures.

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