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Computational modelling of TiO2/SnO2 interfaces for energy storage

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Energy storage devices such as rechargeable lithium-ion batteries are considered as reliable energy storage devices for portable electronic devices, electric vehicles and key enabling devices. This is due to their high energy density, lightweight, long lifetime, environmental benignity and high efficiency. In this work, we make use of hybrid density functional theory to study the electronic properties of (1 1 0) and (1 0 1) TiO2 and SnO2 interfaces. Tin oxide has been considered as one of the most appealing and promising materials with high theoretical capacity for anode materials used for lithium-ion batteries whereas TiO2 provides SnO2 with secondary structure protection in the SnO2/TiO2 interfaces. A detailed analysis was conducted from first principles calculations by making use of plane-wave pseudopotential density functional theory within the generalised approximation for the exchange-correlation functional. It was found that the band positions of both TiO2/SnO2 interfaces change as compared to individual systems and become broader. Also the electronic properties were investigated, i.e. analysis of the total and projected density of states, and charge density differences of the TiO2/SnO2 interfaces. The findings provide a useful information on understanding the interfacial mechanisms for energy storage materials.

Apply to be
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Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

PhD

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