Understanding the Role of Defects in WS_2 layer in contact with ZnO substrate

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The remarkable properties of two-dimensional (2D) materials have garnered significant attention in recent years, and understanding their fundamental behavior is critical for developing next-generation technologies. In this study, we investigate the microscopic behavior of a 2D material, WS_2, with ZnO (1 -1 0 0) taking the role as the substrate as well as charge injection layer in this van der Waals (vdW) heterostructures. Unique combination of tunable optical properties and high carrier mobility of WS_2, as well as ZnO wide band gap, large exciton binding energy and compatibility with existing fabrication technique, provides an attractive outlook for optoelectronic devices. Using density functional theory calculation, we examine the structural and optoelectronic properties of the WS_2/ZnO, including the impact of point defects.

Herein, band alignment of the heterojunction is found to be type I, with the larger band gap in ZnO, which is desirable for using ZnO as an electron injector for radiative recombination in monolayer WS2 forming the active layer in a light-emitting device.

We systematically explore different point defects on our system (V_S, V_W, V_O, V_{Zn}, and O_S) in different strategic positions, cluster defect (V_{WS3}), as well as interstitial (H_i). Our results demonstrate defects influence on modulating the electronic properties of the interface, including band alignment, doping level and charge transfer. This is also reflected by the variety of work function (ϕ) resulted by the presence of each defect. Furthermore, the charged defect analysis allows a deeper understanding on the effect towards the doping description of the material. These insights give crucial information for the design and optimization of devices based on 2D materials, and offer a pathway for enhancing their performance in a wide range of applications.