Supplemental material to the article

Modulation of band gap by normal strain and an applied electric field in SiC-based heterostructures

Note 1. Band structures of the WS_2/SiC vdW heterostructures with different interlayer distances. In order to investigate normal strain influences on electronic structures, we plot the band structures of the WS_2/SiC vdW heterostructures with different interlayer distances (Supplementary Fig. 1). As shown in Supplementary Figs. 1a and b, with a compressive strain, the

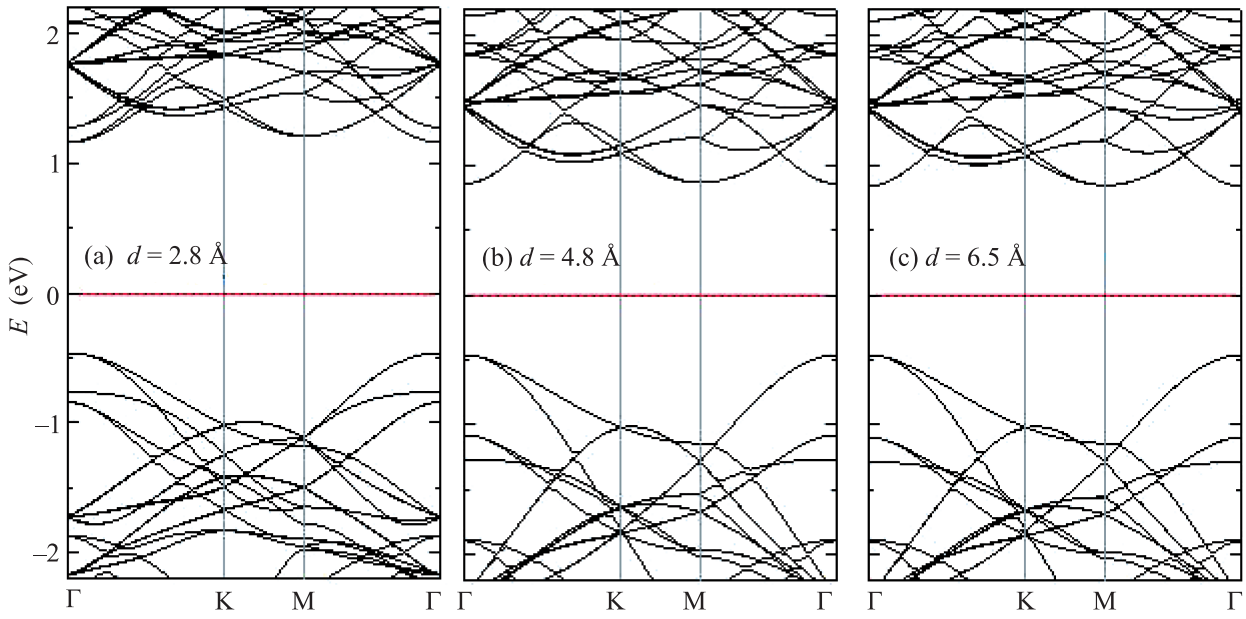

Figure 1: (Color online) The band structures of the WS_2/SiC vdW heterostructures with different interlayer distances. The Fermi levels are marked by the red dashed line

band gap gets gradually larger as the interlayer distance decreases. In contrast, from Supplementary Figs. 1b and c, as the system is under a tensile strain, the band gap keeps almost the same due to the weakening vdW interaction. It implies that the band gap of the WS_2/SiC vdW heterostructures is sensitive to the compressive strain.

Note 2. The PDOS of WS_2/SiC vdW heterostructures under different E-field strength. As shown in Supplementary Figs. 4e–h, in the presence of the positive field, the states at the top of the valence band are due to the p-electrons of C, and those at bottom of the conduction band are owned to the d-electrons of W and p-electrons of S. Under the influence of the negative E-field, the p-electrons of S and the d-electrons of W contribute to the modification of CBM, which crucially induce the increasing variations in the band gap, as shown in Supplementary Figs. 4 c–e. By contrast, the narrowing of band gap are mainly due to the p-electrons of Si at bottom of the conduction band and partly due to the d-electrons of W and p-electrons of S in the top of the valence band, as shown in Supplementary Figs. 4a and b.

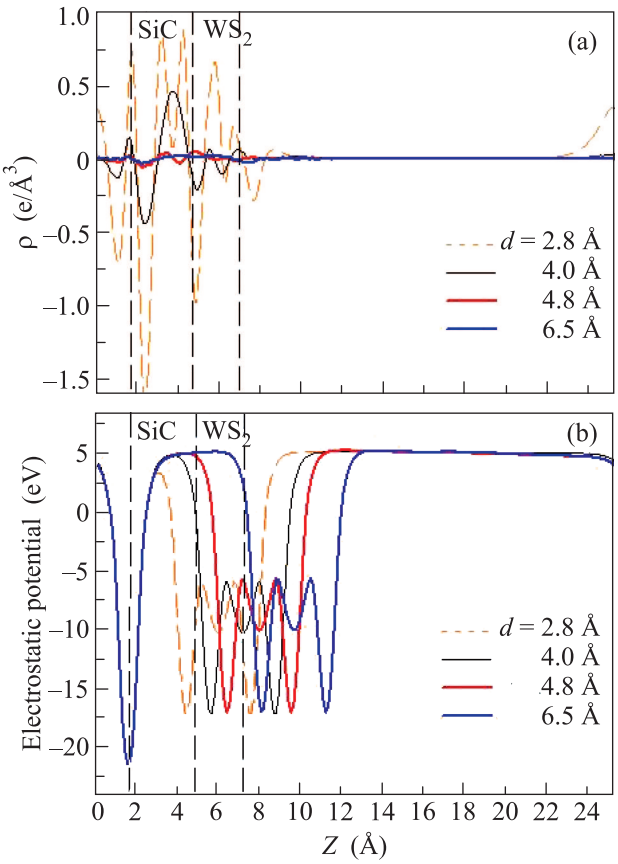

Figure 2: (Color online) (a) – Electrostatic potentials and (b) – plane-averaged charge density differences of the WS_2/SiC vdW heterostructures with different interlayer distances

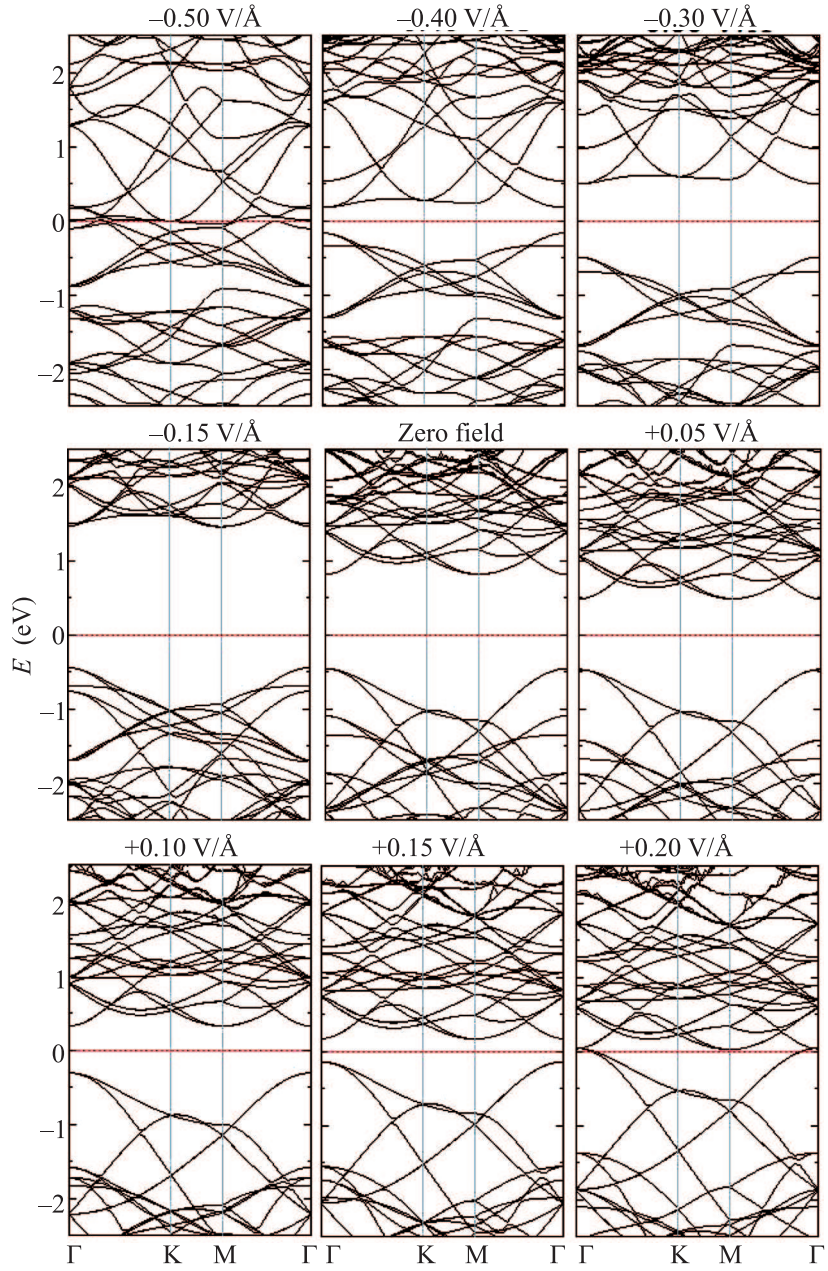

Figure 3: (Color online) The band structures of the WS_2/SiC vdW heterostructures with different E-field strength. The Fermi levels are marked by the red dashed line

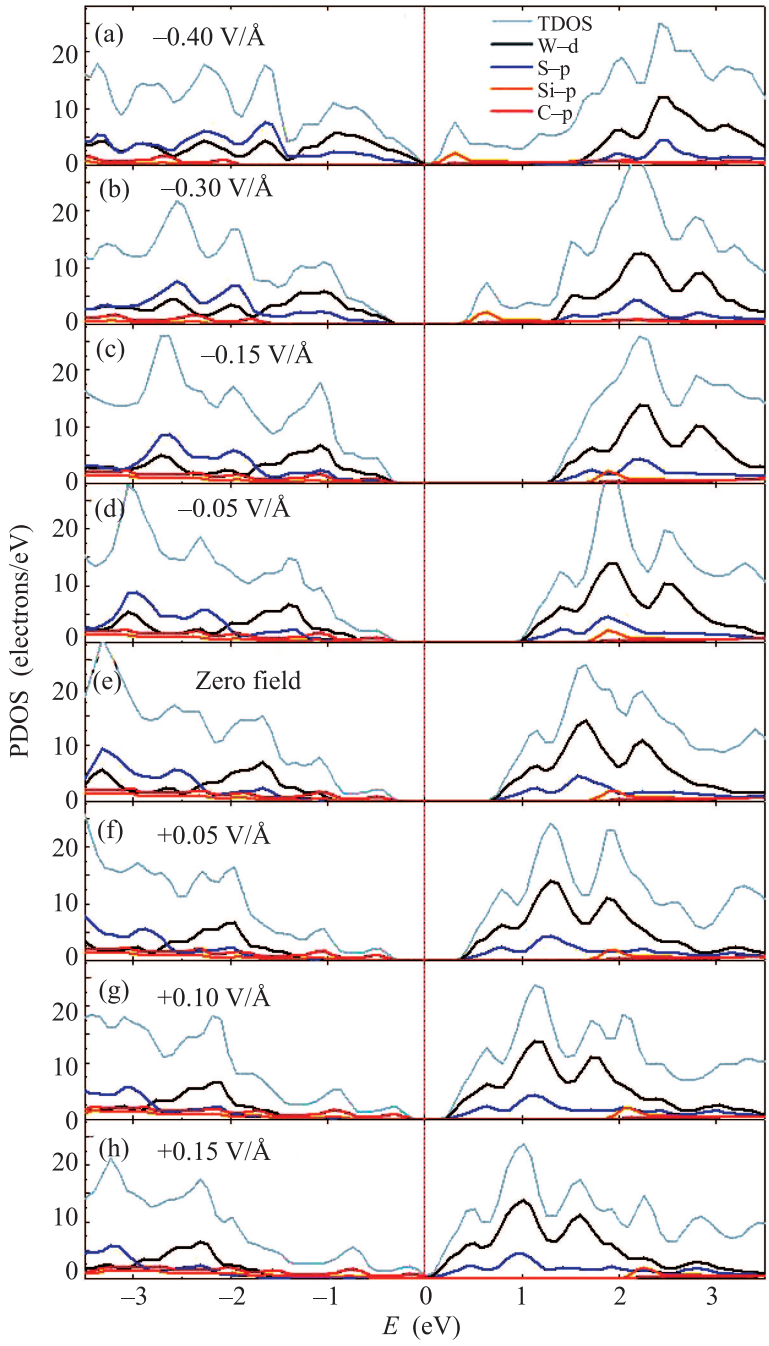

Figure 4: (Color online) PDOS of the WS_2/SiC vdW heterostructures with different E-field strength. The Fermi level is marked by the red dashed line