Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Structures and characteristics of atomically thin ZrO_2 from monolayer to bilayer and two-dimensional ZrO_2-MoS_2 heterojunction

Junhui Weng and Shang-Peng Gao*

Department of Materials Science, Fudan University, Shanghai 200433, P. R. China. E-mail: gaosp@fudan.edu.cn

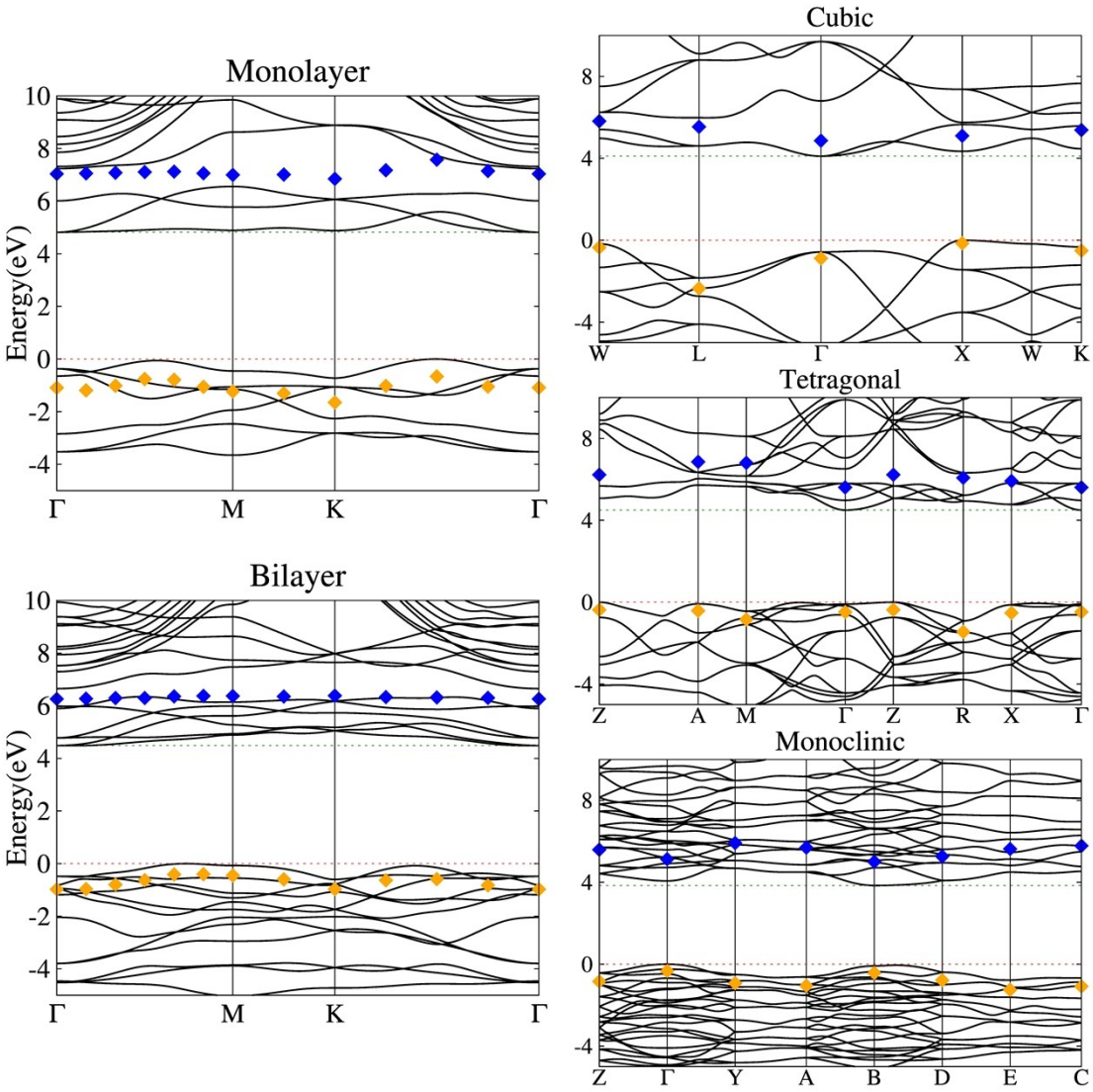

Figure S1 Electronic band structures calculated by DFT-GGA using ABINIT code for 2D and bulk ZrO_2 polymorphs: (a) monolayer ZrO_2, (b) bilayer ZrO_2, (c) cubic ZrO_2, (d) tetragonal ZrO_2, and (e) monoclinic ZrO_2. Yellow points and blue points indicate the values of highest valence band energies and lowest conduction band energies obtained with the GW method, respectively. The valence band maximum from the DFT-GGA calculation is set to 0 eV.

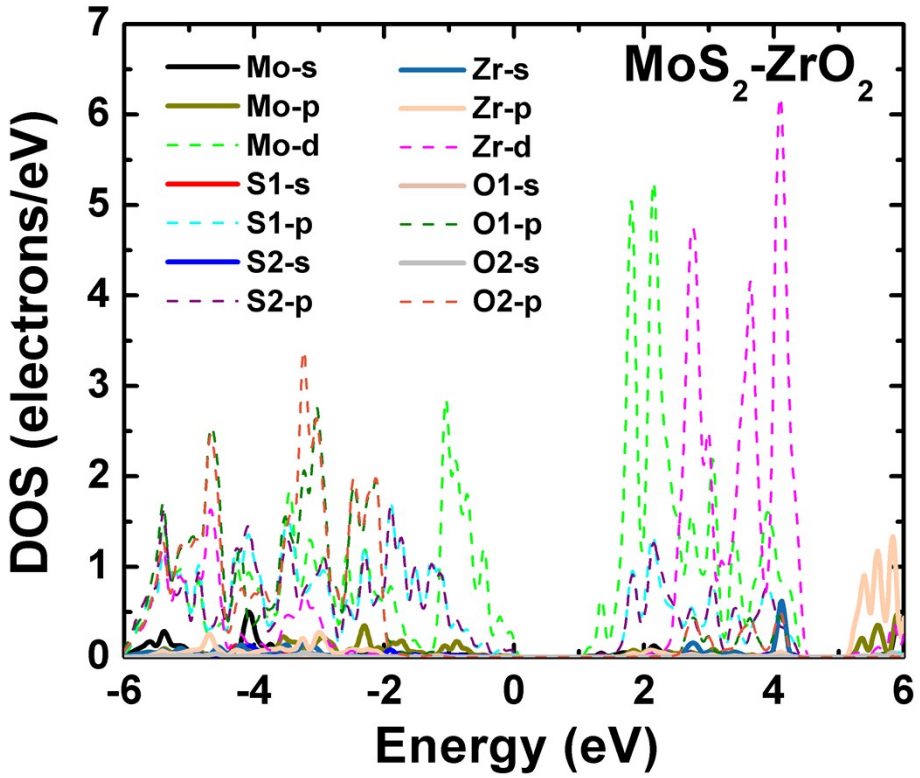

Figure S2 The calculated PDOS of 2D ZrO_2-MoS_2 heterojunction. The dotted lines indicate the PDOSs which are more significant and have been shown in the main text, and the solid lines shows the less significant PDOSs for completeness and comparison.