Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Realizing Semiconductor to Metal Transition in Graphitic ZnO and MoS_2 Nanocomposite with External Electric Field

Weihua Wu,[†] Shaobin Tang,*[,†] Junjing Gu[‡], and Xinrui Cao[§,∥]

[†]Key Laboratory of Organo-Pharmaceutical Chemistry of Jiangxi Province, Gannan Normal University, Ganzhou 341000, China
[‡]State Key Laboratory of Physical Chemistry of Solid Surfaces and Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China
[§]Department of Theoretical Chemistry and Biology, School of Biotechnology, Royal Institute of Technology, S-106 91 Stockholm, Sweden

[∥] Department of Physics and Institute of Theoretical Physics, Xiamen University, Xiamen 361005, China

*Corresponding author e-mail: tsb1980@xmu.edu.cn

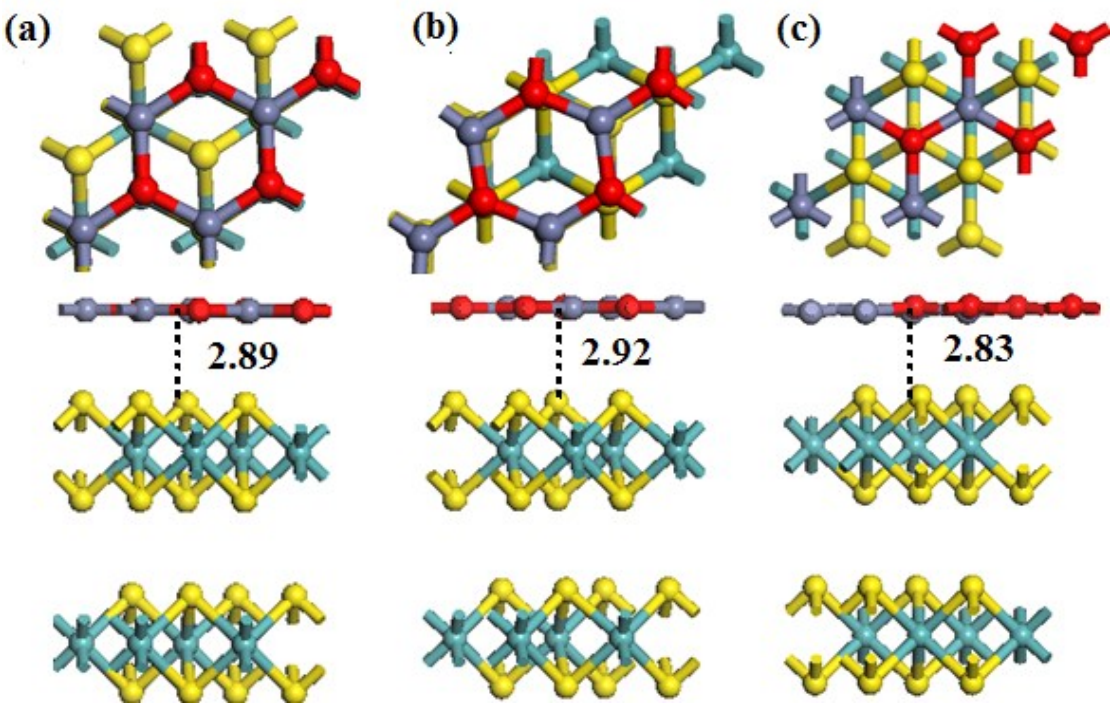

Figure S1. Top and side view of geometrical structures of g-ZnO/two-MoS_2 with (a) AA, (b) AB-Zn, and (c) AB-O stacking patterns. The distance is in Å.

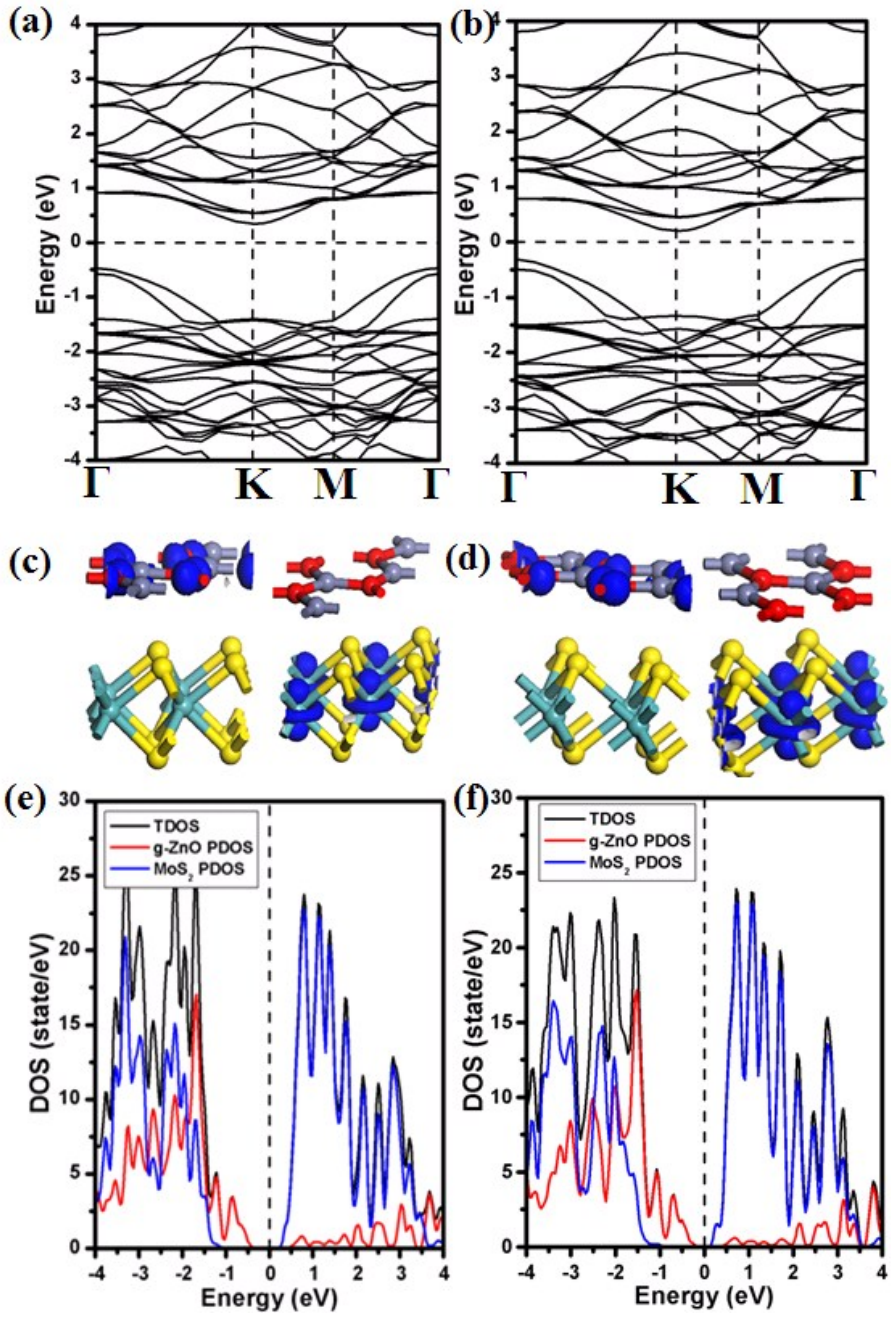

Figure S2. (a, b) Band structures, (c, d) partial charge densities of VBM (left panel) and CBM (right panel), and (e, f) TDOS and PDOS of g-ZnO and MoS_2 for g-ZnO/MoS_2 with (a), (c) and (e) AB-Zn-2, and (b), (d), and (f) AB-O-2 stacking patterns. The isosurfaces in (c, d) are 0.04 e/Å^3, and the Fermi level is set to 0.

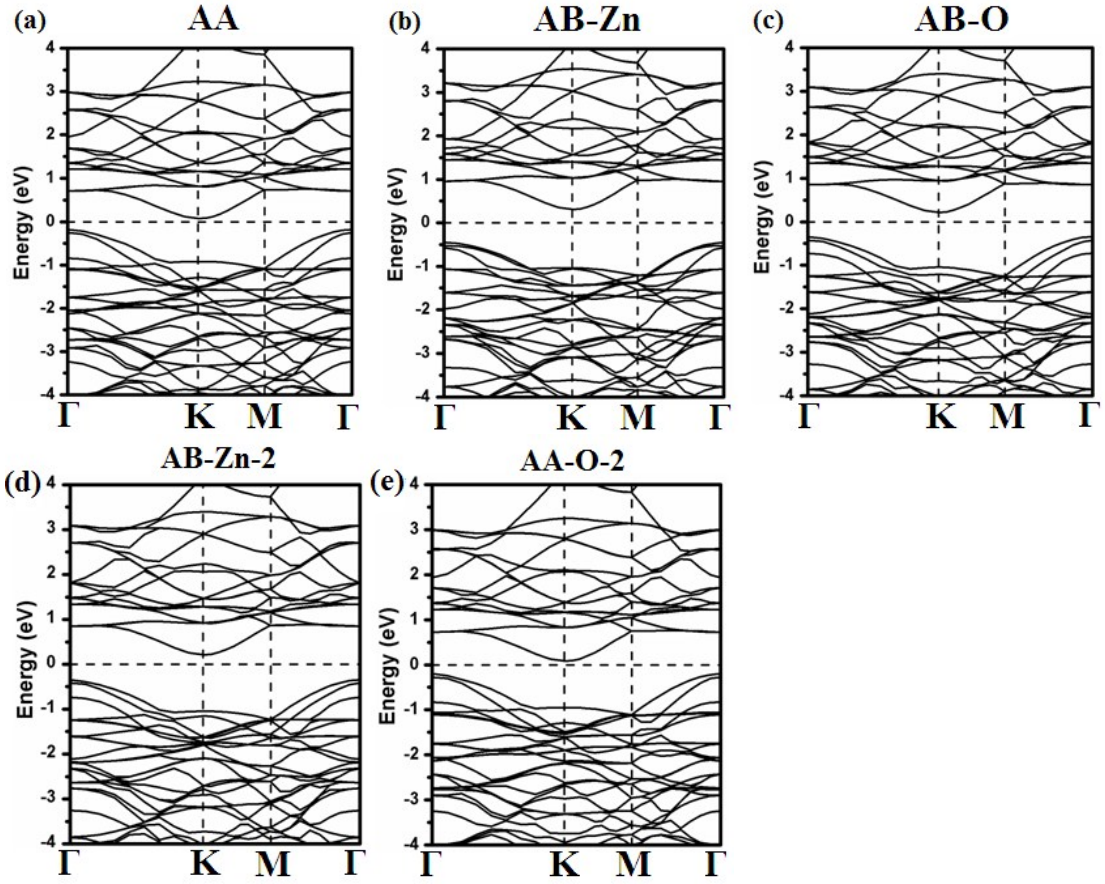

Figure S3. Band structures of g-ZnO/MoS_2 with lattice constant of isolated g-ZnO for different configurations. The Fermi level is set to 0.

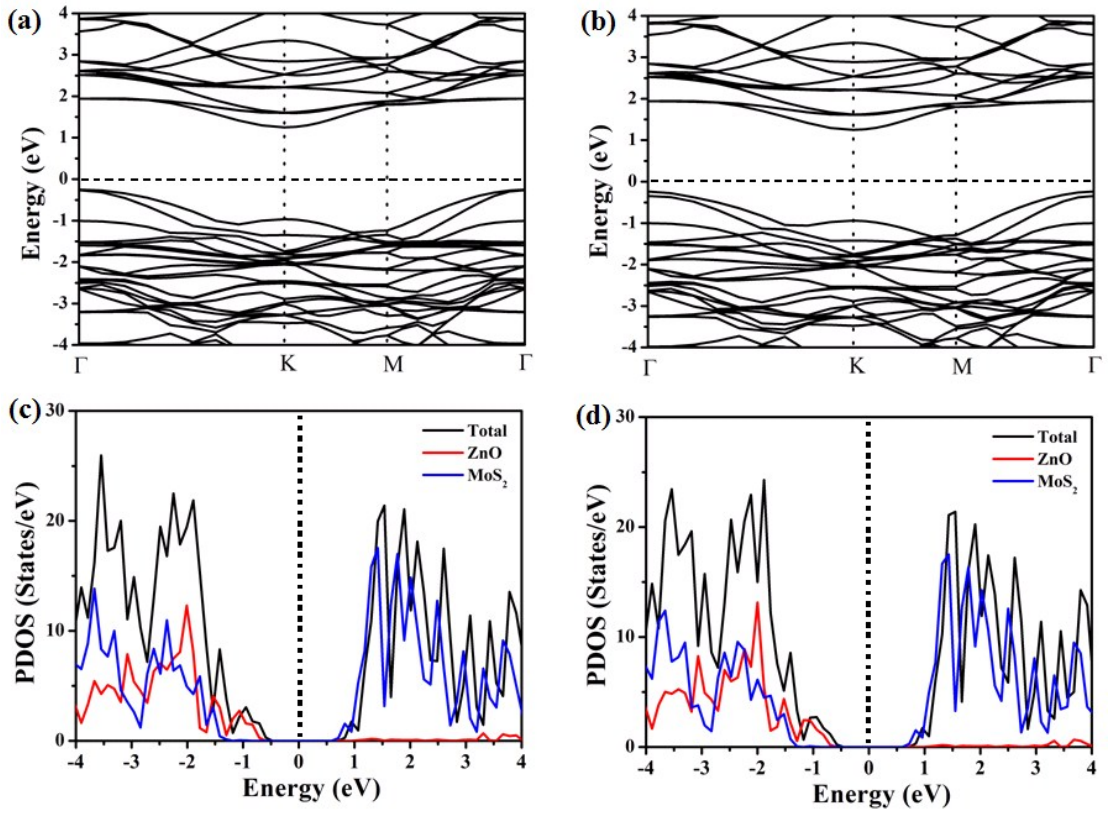

Figure S4. The band structures and PDOS of g-ZnO/MoS_2 by HSE06. (a) and (c) AA, and (b) and (d) AB-O-2 configurations. The Fermi level is set to 0.

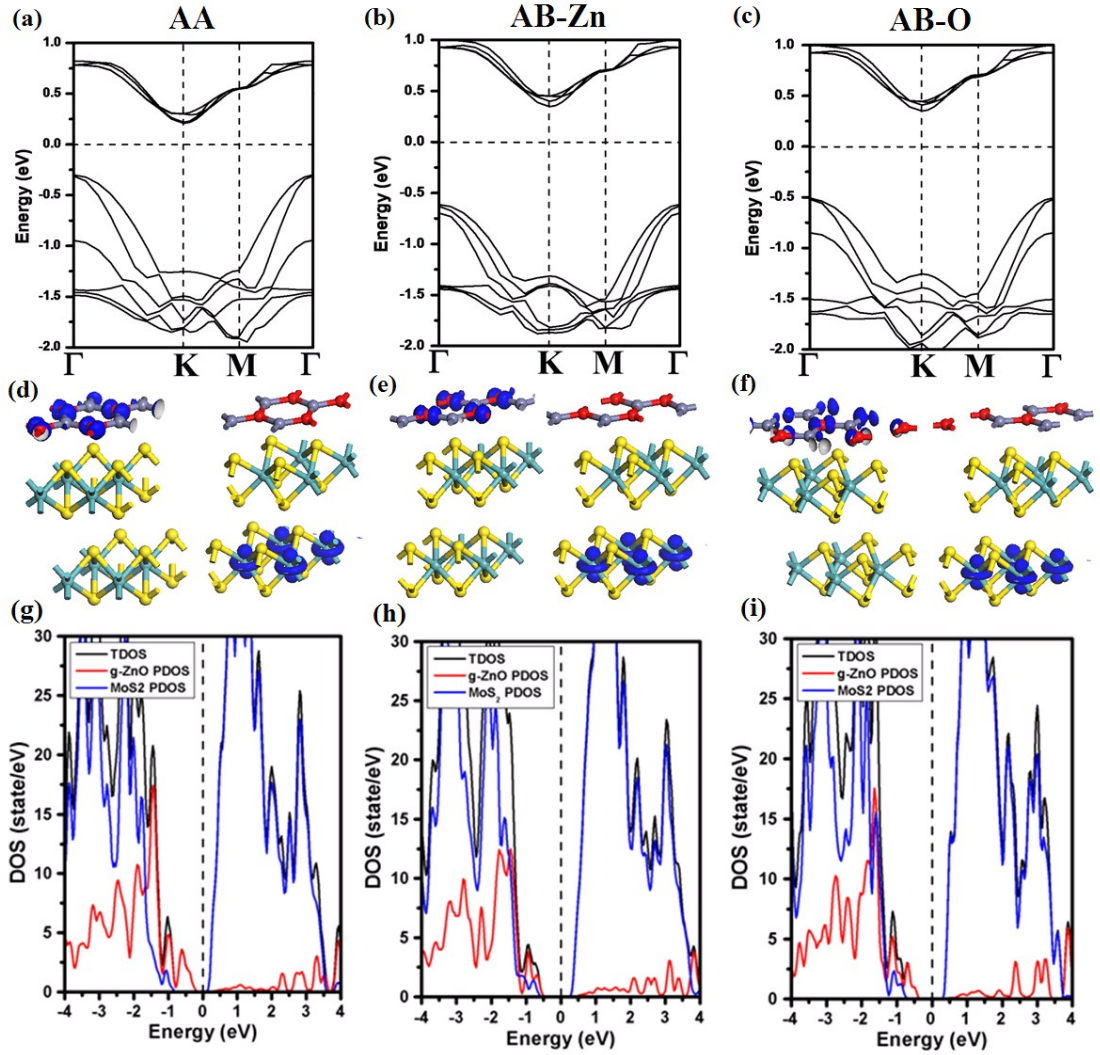

Figure S5. (a)-(c) Band structures, (d)-(f) partial charge densities of VBM (left panel) and CBM (right panel), and (g)-(i) TDOS and PDOS of g-ZnO and bilayer MoS_2 for g-ZnO/two-MoS_2 with (a), (d) and (g) AA, (b), (e), and (h) AB-Zn, (c), (f), and (i) AB-O stacking patterns. The isosurfaces in (d)-(f) are 0.003 e/Å^3, and the Fermi level is set to 0.

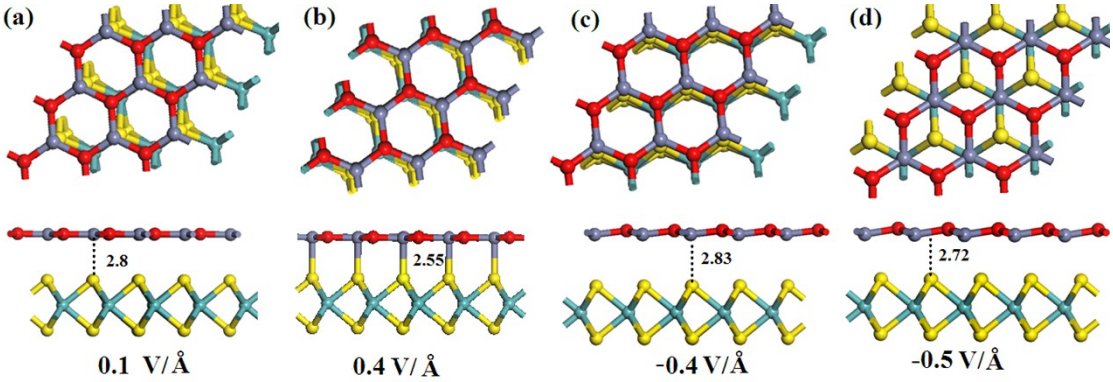

Figure S6. Top and side view of geometrical structures of g-ZnO/MoS_2 with initial AA configuration under the E-field with different strength. The distance is in Å.

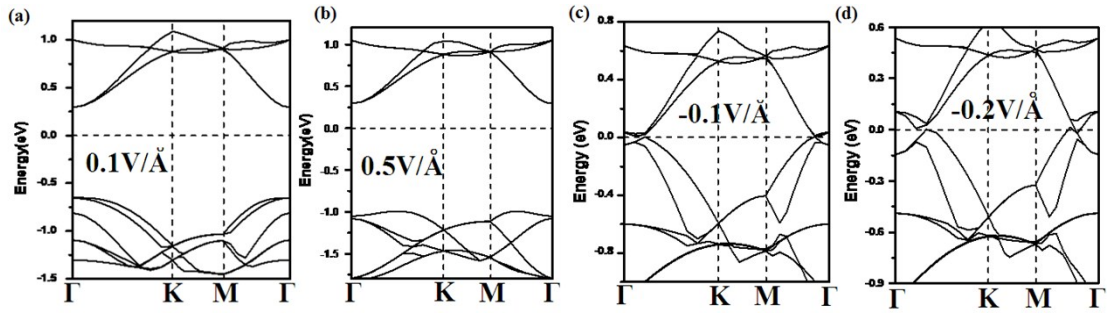

Figure S7. Band structures of g-ZnO/MoS_2 with initial AA stacking pattern under the external electric field with different strength. The Fermi level is set to 0.

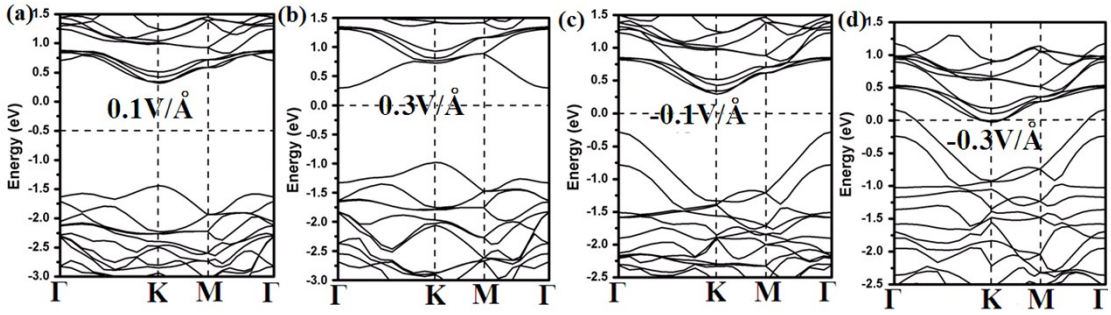

Figure S8. Band structures of g-ZnO/MoS_2 with lattice constant of isolated MoS_2 for AB-O stacking pattern under the external electric field with different strength. The Fermi level is set to 0.