Supporting Information

Controlling of the Electronic Properties of WS_2 by Graphene Oxide Substrate from First-principles calculations

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Table S1. Band gaps of pristine WS_2 and some GO/WS_2 heterostructures with and without considering SOC effect.

Band Gap/eV	WS_2	WS_2/GO-h_2e (8%)	WS_2/GO-h_2e (40%)	WS_2/GO-h_2e (56%)	WS_2/GO-h_2e (80%)
PBE	1.92	0.32	1.29	1.72	1.91
PBE+SOC	1.58	0.33	1.15	1.48	1.57

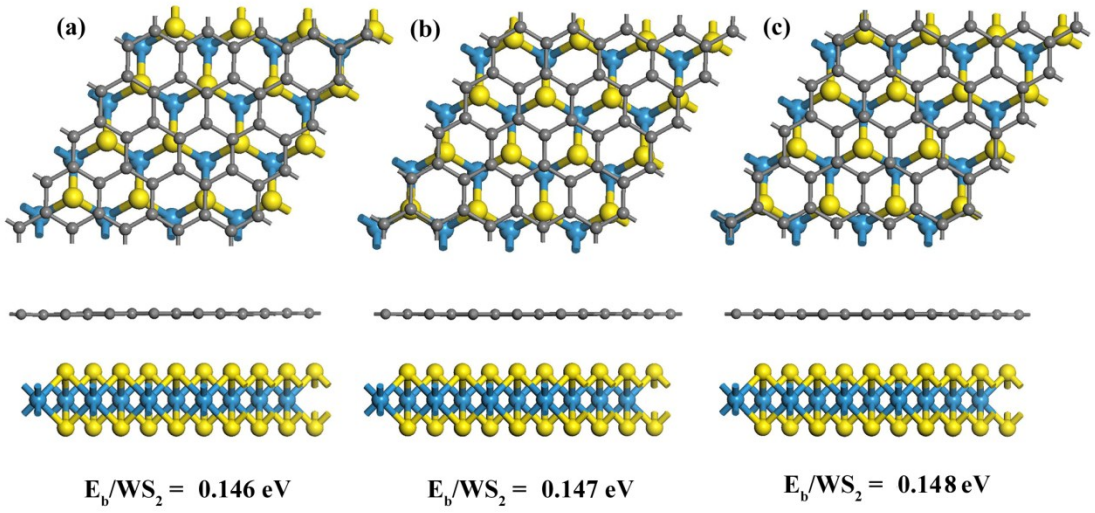

Fig. S1. Different staking patterns and the binding energies per WS_2 unit of graphene and WS_2 hybrids.

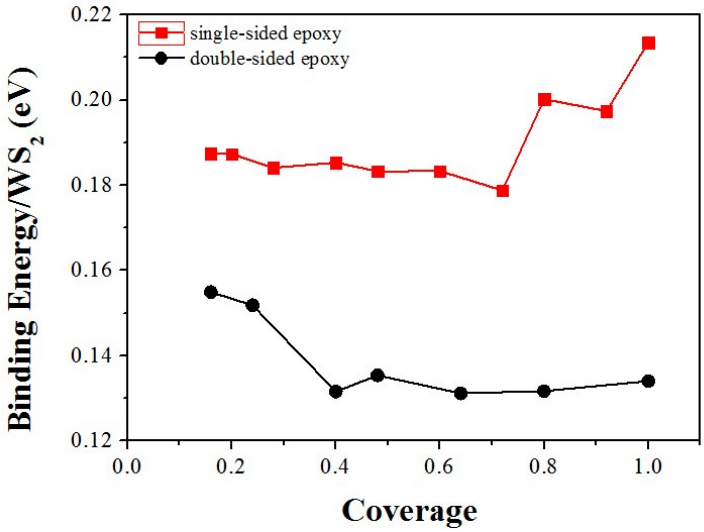

Fig. S2. Binding energies of WS_2 and GO with epoxy distributed on single side and on both sides heterostructures.

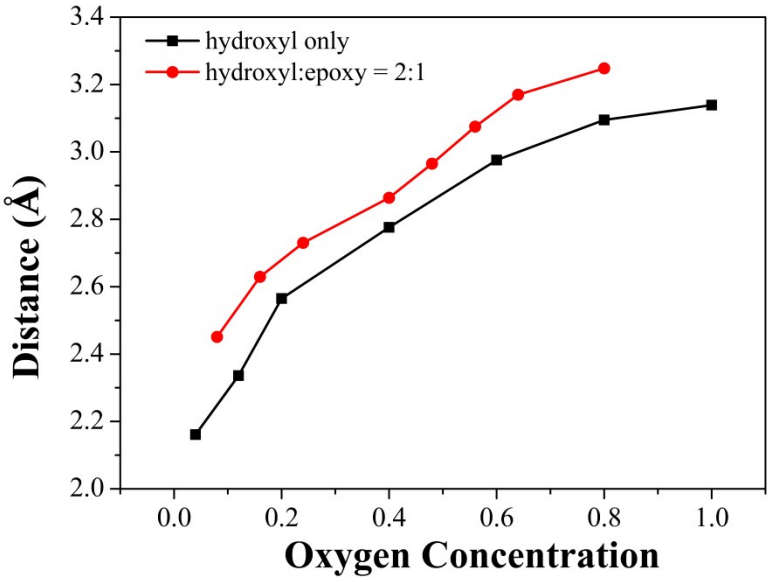

Fig. S3. The distances between S atoms in WS_2 and O atoms in GO as the function of oxygen concentration.

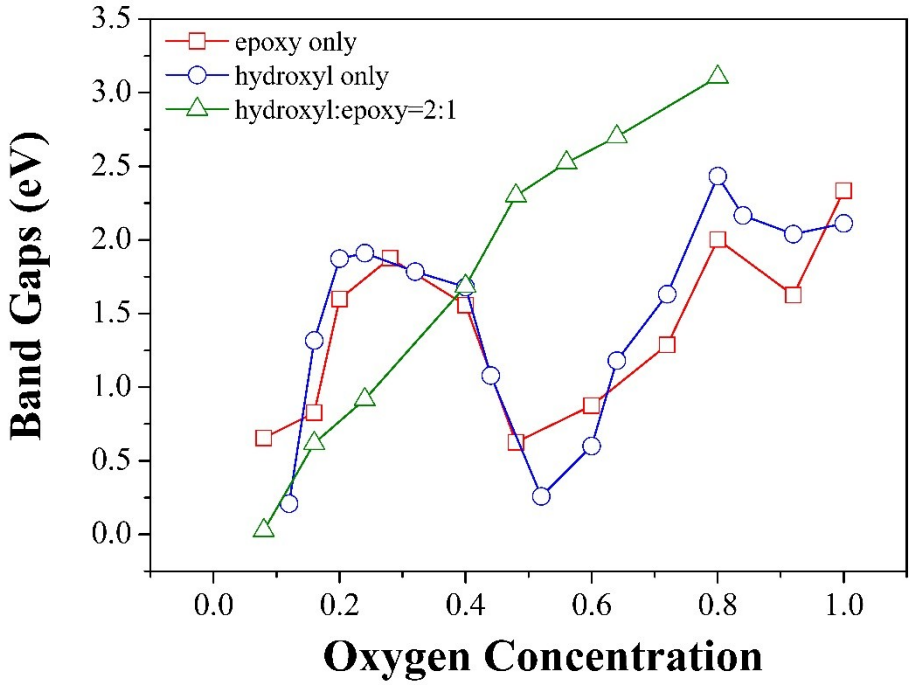

Fig. S4. Band gaps of the free-standing graphene oxide as the oxygen concentration increasing.

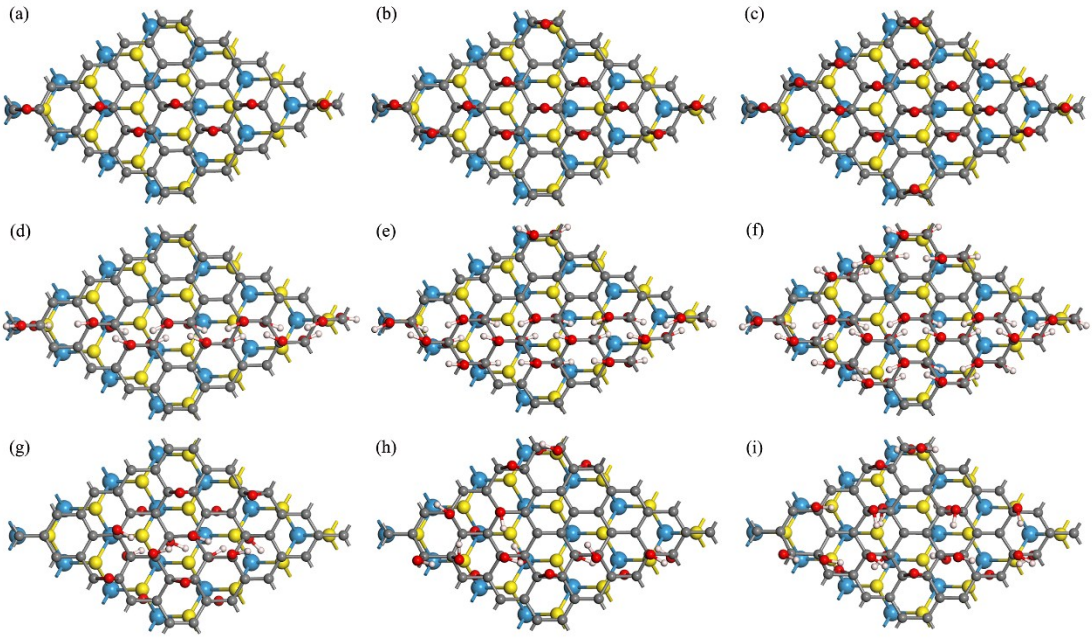

Fig. S5. Optimized Structures of GO and WS_2 heterostructures. (a) to (d) are the structures of e-GO/WS_2 (h_2-GO/WS_2) at the first peak, the peak valley and the second peak of the band gaps. Their oxygen concentrations are 0.28 (0.32), 0.48 (0.52) and 0.72 (0.72), respectively. (g) to (i) are the heterostructures with the same oxygen concentration of 0.48 but with different hydroxyl to epoxy ratios of 1:1, 2:1 and 4:1, respectively.