Electronic Supplementary Information (ESI) for

Band Gap Opening of Bilayer Graphene by Graphene oxides Support Doping

Shaobin Tang,*,† Weihua Wu,† Xiaojun Xie,⊥ Xiaokang Li, *,† and Junjing Gu‡

†*Key Laboratory of Organo-Pharmaceutical Chemistry of Jiangxi Province, Gannan Normal University, Ganzhou 341000, China*
⊥*School of physics and electric information, 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*
**Correspondence authors* e-mail: *tsb1980@xmu.edu.cn*

Table S1: The charge transfer Δq (e) from GOs to its neighboring graphene layer as a function of the sampling k-points.

structure	7×7	9×9	11×11
BG/GO-2OH-2	-0.03/0.03	-0.03/0.02	-0.03/0.02
BG/GO-O-2OH-1	-0.03/0.0	-0.03/0.0	-0.04/0.0
BG/GO-O-2OH-2	-0.02/0.02	-0.02/0.01	-0.02/0.02

Table S2: Summary of calculated results for bilayer graphene (BG) supported on other GOs: the adsorption energy per carbon atom of graphene layer E_b (in meV), the minimum distance d_1 (in Å) between GOs and its neighboring graphene layer, the distance d_2 (in Å) of BG, and the band gap E_g (in meV) in BG. The corresponding structures are shown in Fig. S1.

structure	E_a	d_1	d_2	E_g
BG/GO-2O-a	-31	3.08	3.14	199
BG/GO-2O-b	-31	3.08	3.14	199
BG/GO-2OH-2a	-28	2.64	3.3	94
BG/GO-2OH-2b	-27	2.59	3.13	40
BG/GO-O-2OH-2a	-27	2.79	3.38	176
BG/GO-2O-2OH-2b	-37	3.05	3.33	254
BG/GO-2O-4OH-1a	-40	2.53	3.31	49
BG/GO-2O-4OH-2a	-37	2.77	3.39	263
BG/GO-2O-4OH-2b	-38	2.75	3.38	157

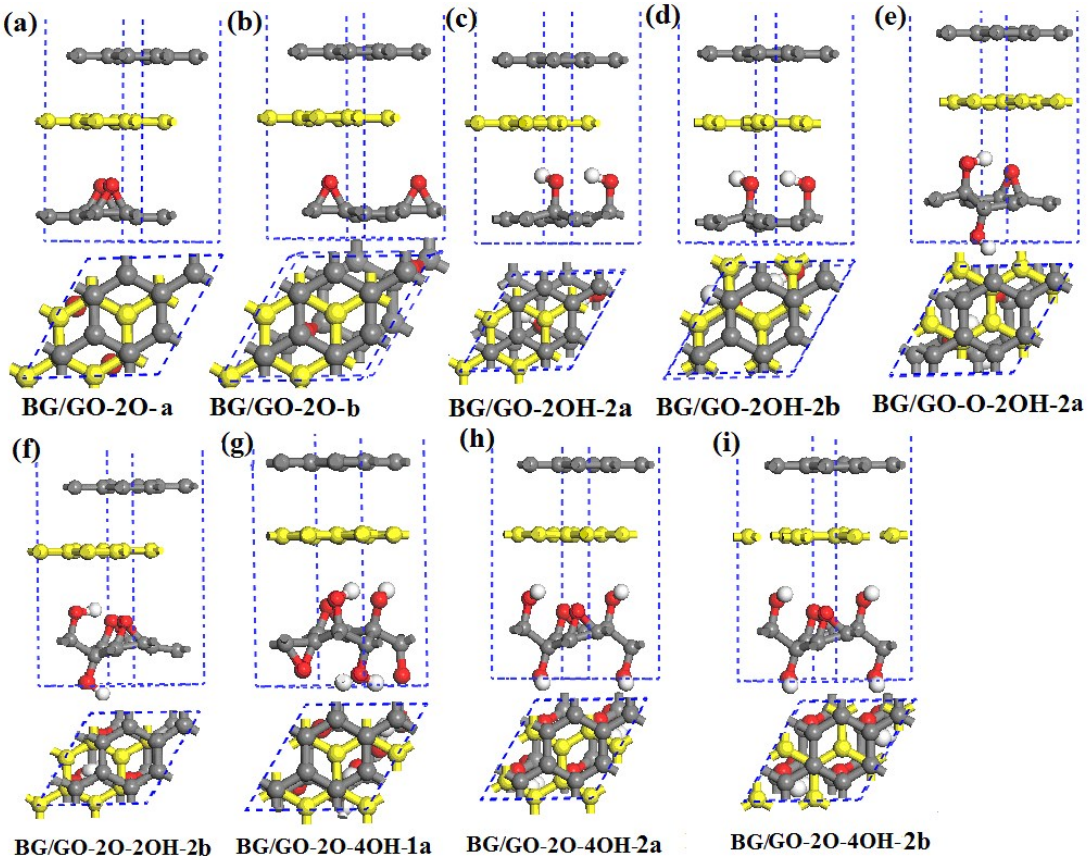

Fig. S1 Side and top view of optimized structures of BG/GOs for other stacking order. The yellow balls represent the bottom graphene layer.

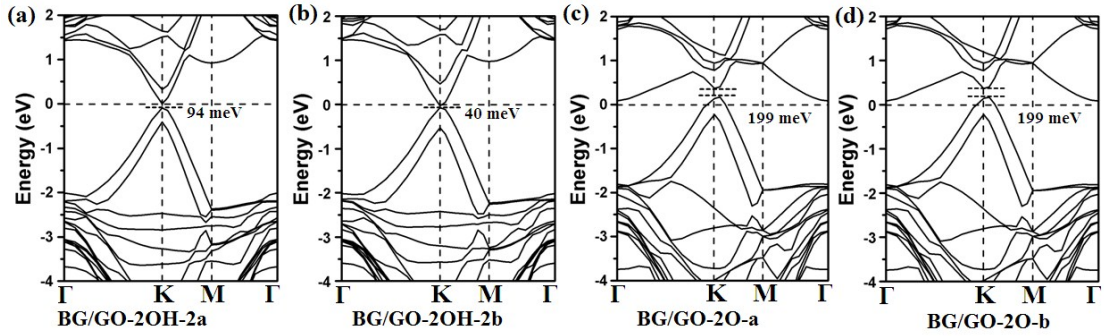

Fig. S2 Band structures of BG/GOs only containing single the hydroxyl and epoxy groups. The Fermi level is set to 0. The corresponding geometry structures are shown in Figs. S1(a)-(d)

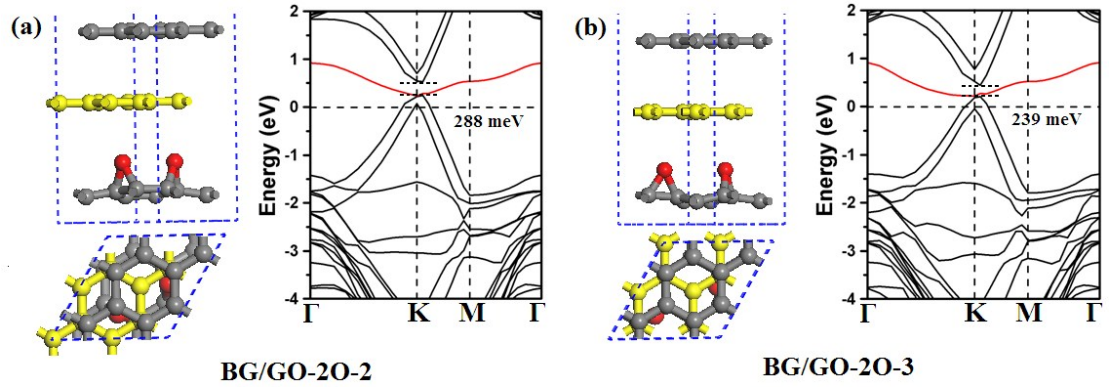

Fig. S3 Side and top view of optimized structures of BG/GOs for other atomic arrangement of two adsorbed epoxides on substrate (left panel) and the corresponding band structures (right panel). The band marked in red represent the doped state contributed by GOs. The Fermi level is set to 0.

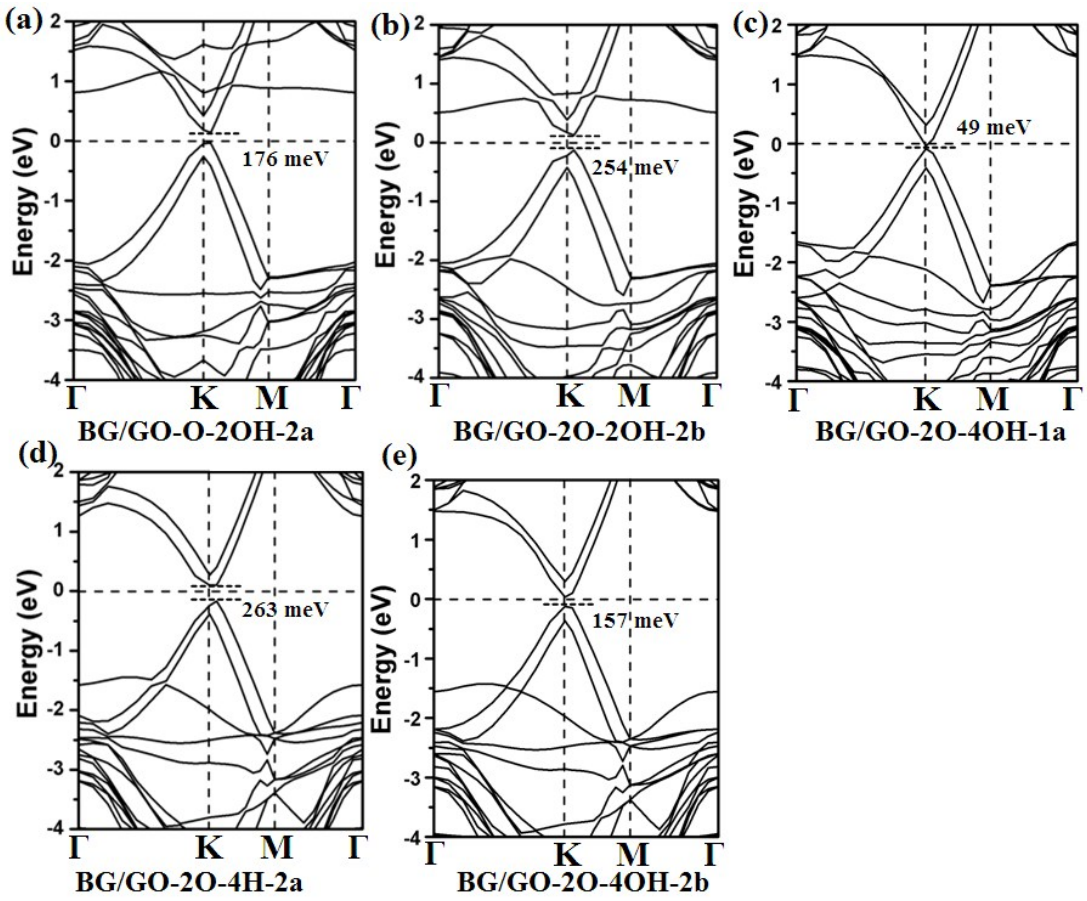

Fig. S4 Band structures of BG/GOs containing both the hydroxyl and epoxy groups for other stacking pattern. The Fermi level is set to 0. The corresponding geometry structures are shown in Figs. S1(e)-(i).

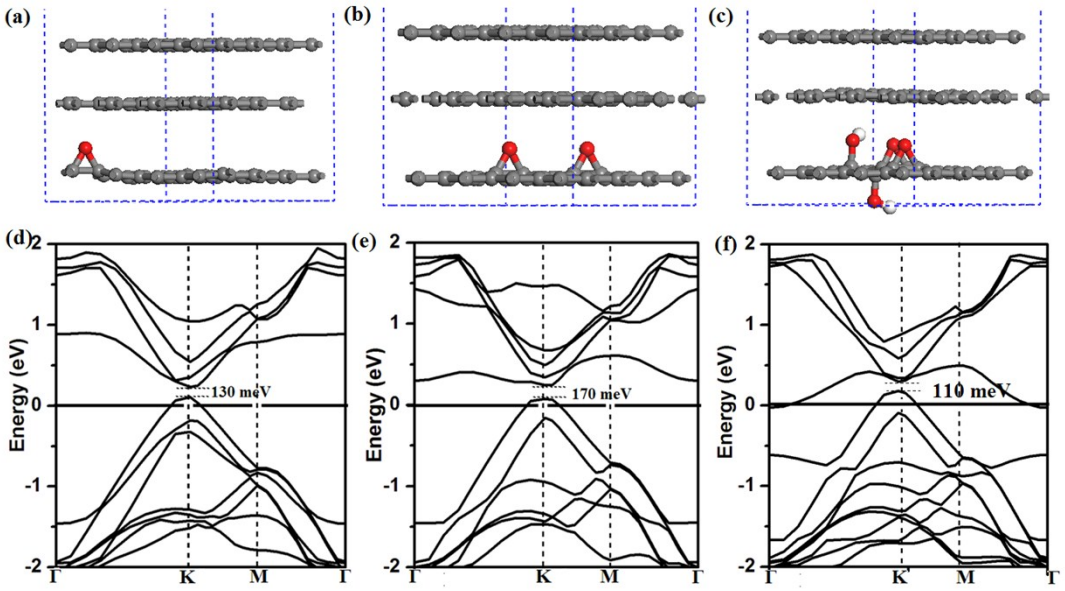

Fig. S5. Optimized structures (a-c) and band structures of (d-f) of BG/GOs with low oxidation concentration. (a) and (d) One epoxide, (b) and (e) two epoxides, and (c) and (f) one hydroxyl group and two epoxides. The Fermi level is set to 0.