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Distribution of oxygen functional groups of graphene oxide obtained from low-temperature atomic layer deposition of titanium oxide

Dong Seok Shin,†,[a] Hyun Gu Kim,†,[b] Ho Seon Ahn,†,[c] Hu Young Jeong,[d] Yeon Jung Kim,[e] Dorj Odkhuu,[a] N. Tsogbadrakh,[f] Han-Bo-Ram Lee*,[b] and Byung Hoon Kim*,[a]

[a.] *Department of Physics, Incheon National University, Incheon 22012, Republic of Korea. E-mail: kbh37@inu.ac.kr*

[b.] *Department of Materials Science and Engineering, Incheon National University, Incheon 22012, Republic of Korea. E-mail: hbrlee@inu.ac.kr*

[c.] *Department of Mechanical Engineering, Incheon National University, Incheon 22012, Republic of Korea.*

[d.] *UNIST Central Research Facilities (UCRF) and School of Materials Science and Engineering, UNIST, Ulsan 44919, Republic of Korea.*

[e.] *Department of Marine Science, Incheon National University, Incheon 22012, Republic of Korea.*

[f.] *Department of Physics, National University of Mongolia, Ulaanbaatar 14201, Mongolia*

† These author contributed equally to this work.

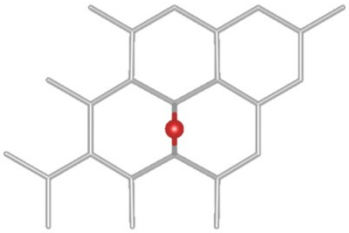
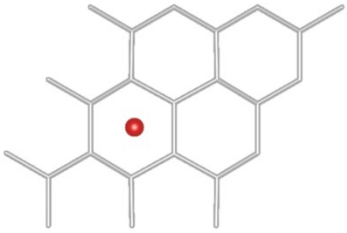
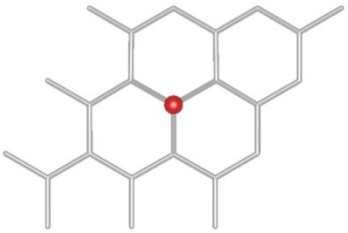
	Bridge-site	Hollow-site	Top-site
Top -View			
Side -View			
E_b	-2.48 eV		-2.23 eV

FIG. S1: The top and side views of the adsorption sites of a single epoxide functional group on graphene: bridge, hollow, and top sites. Red sphere denotes the oxygen atom. The corresponding binding energies E_b are shown at the bottom. The bridge-site is the most stable and the hollow-site exhibit the positive binding energy, which indicates an unfavorable adsorption.

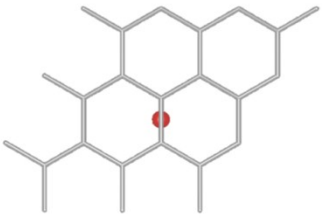
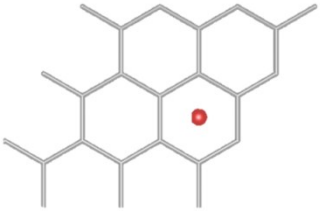
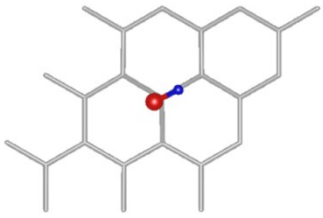
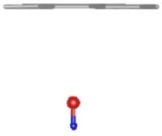
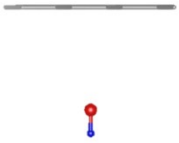
	Bridge-site	Hollow-site	Top-site
Top -View			
Side -View			
E_b			-2.36 eV

FIG. S2: The top and side views of the adsorption sites of a single hydroxyl functional group on graphene: bridge, hollow, and top sites. Red and blue spheres denote the oxygen and hydrogen atoms, respectively. The corresponding binding energies E_b are shown at the bottom. The hydroxyl groups adsorb onto the graphene sheet only with the top-site.

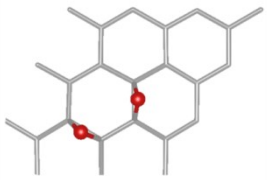
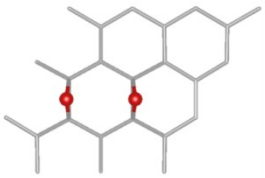
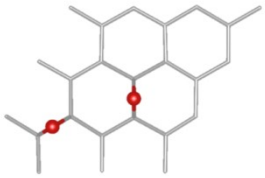
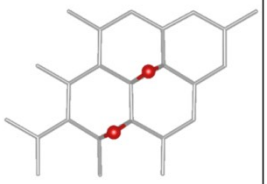
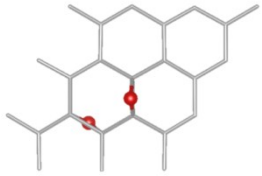
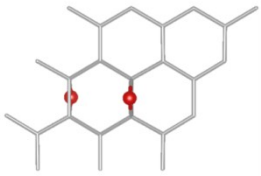
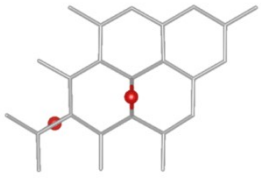
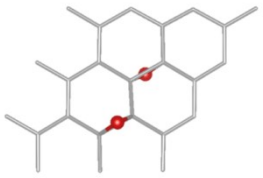
	Type-1 (meta)	Type-2 (para)	Type-3	Type-4
Top -View	one-side			
				
E_b	-2.61 eV	-2.27 eV	-2.30 eV	-2.48 eV
Top -View	two-side			
				
E_b	-2.79 eV	-2.25 eV	-2.37 eV	-2.71 eV

FIG. S3: The top views of the adsorption sites of two epoxide functional groups on graphene. The corresponding binding energies E_b are shown at the bottom. The epoxide groups adsorb on graphene with two-side in close proximity pattern.

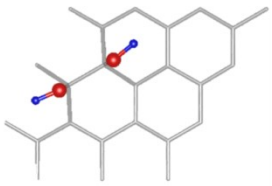
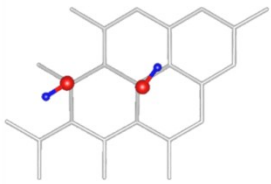
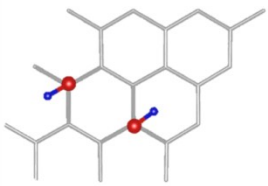
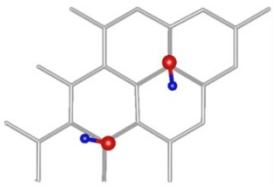
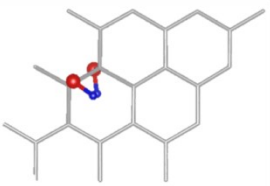
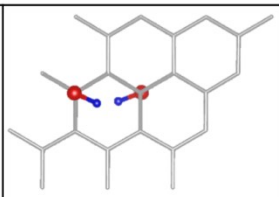
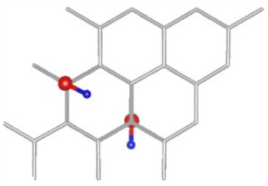
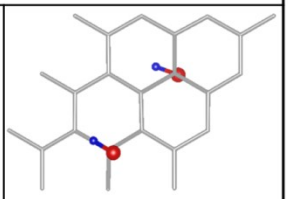
	Type-1 (ortho)	Type-2 (meta)	Type-3 (para)	Type-4
Top -View	One-side			
				
E_b	-2.08 eV	-1.96 eV	-1.61 eV	-1.33 eV
Top -View	Both-side			
				
E_b	-2.67 eV	-2.39 eV	-2.02 eV	-1.53 eV

FIG. S4: The top views of the adsorption sites of two hydroxyl functional groups on graphene. The corresponding binding energies E_b are shown at the bottom. Similar to the epoxide case, the hydroxyl groups adsorb on graphene with two-side in close proximity pattern.

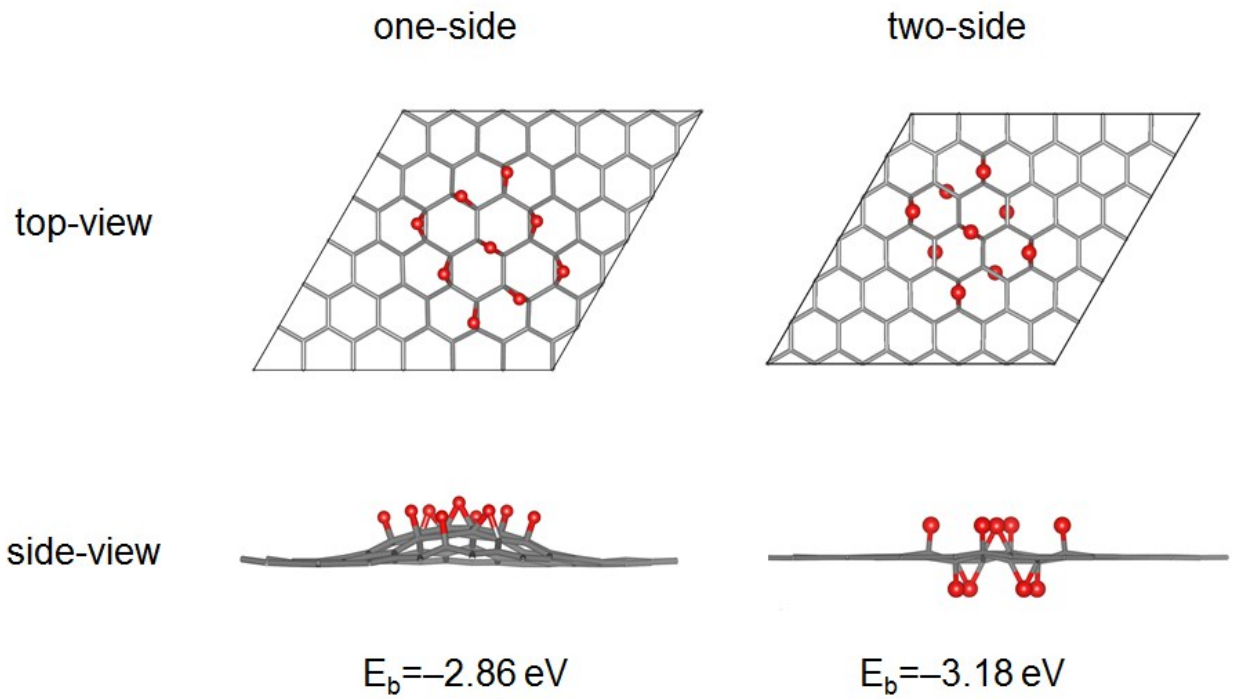


FIG. S5: The top and side views of the one-side and two-side adsorptions of nine epoxide functional groups on graphene. The corresponding binding energies E_b are shown at the bottom. The epoxide groups adsorb onto the graphene with the two-side configuration, which is also the case for the hydroxyl groups (not shown).

TABLE S1: Total energies (eV) of one and nine (eight) epoxide (hydroxyl) functional groups on graphene for the spin-polarized and spin-non-polarized calculations. Those for the pristine graphene and the isolated O and H atoms in a vacuum are also listed.

Systems	Spin-polarized		Spin-non-polarized	
	uniform	domain	uniform	domain
1-epoxide/graphene	-668.301		-668.300	
1-hydroxyl/graphene	-672.027		-672.032	
9-epoxide/graphene	-703.852	-706.836	-703.852	-706.836
8-hydroxyl/graphene	-733.029	-740.299	-733.028	-740.299
pristine graphene	-664.399		-664.399	
oxygen	-1.534		-0.472	
hydrogen	-1.113		-0.188	