

Supplementary Information (SI)

Epoxy-Carbonyl Conformation of Graphene Oxides

U. Kushan Wijewardena,^a Shirnece E. Brown,^b and Xiao-Qian Wang^{*a}

^a Department of Physics and Center for Functional Nanoscale Materials, Clark Atlanta University, Atlanta, Georgia, 30314, USA. E-mail: xwang@cau.edu

^b Department of Chemistry and Center for Functional Nanoscale Materials, Clark Atlanta University, Atlanta, Georgia, 30314, USA.

Table S1. Lattice parameters of epoxy-carbonyl combination

a (Å)	b (Å)	c (Å)	α (degree)	β (degree)	Γ (degree)
5.88	4.22	23.98	91.24	90.31	87.58

Table S2. Fractional coordinates of epoxy-carbonyl combination

Atom No:	Element	Fractional coordinates of Atoms		
		x	y	z
C1	C	0.7950	0.6396	0.4959
C2	C	0.2020	0.9413	0.5082
C3	C	0.2098	0.6107	0.4988
C4	C	0.7965	0.9539	0.4742
C5	C	0.6325	0.0681	0.4153
C6	C	0.4200	0.3948	0.4956
C7	C	0.9977	0.1149	0.4916
C8	C	0.9999	0.4576	0.4947
O1	O	0.6622	0.9491	0.3565
O2	O	0.4643	0.3022	0.4236
O3	O	0.3899	0.1068	0.5317
O4	O	0.6128	0.5229	0.5291

Table S3. Bond lengths of epoxy-carbonyl combination

Bonding Atoms	Bond Length (Å)
C1-C4	1.41
C1-C8	1.40
C1-O4	1.38
C2-C3	1.39
C2-C7	1.41
C2-O3	1.38
C3-C6	1.51
C3-C8	1.42
C4-C5	1.52
C4-C7	1.41
C5-O2	1.38
C5-O1	1.21
C6-O2	1.42
C6-O3	1.44
C6-O4	1.39
C7-C8	1.44

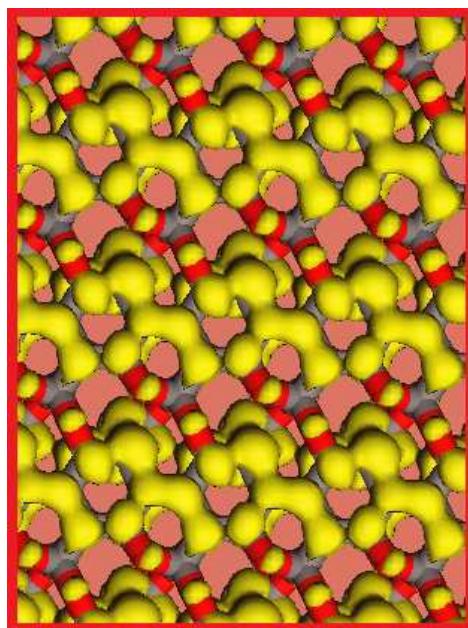


Fig. S1. Simulated STM image of epoxy-carbonyl combination.

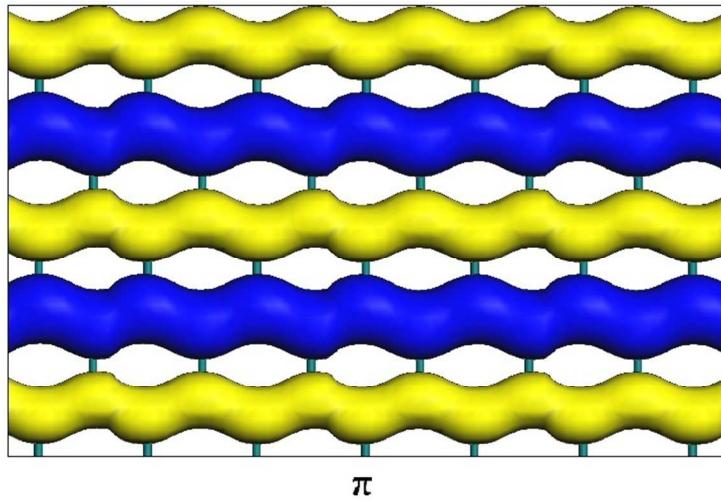


Fig. S2. Charge densities of the π state in graphene.

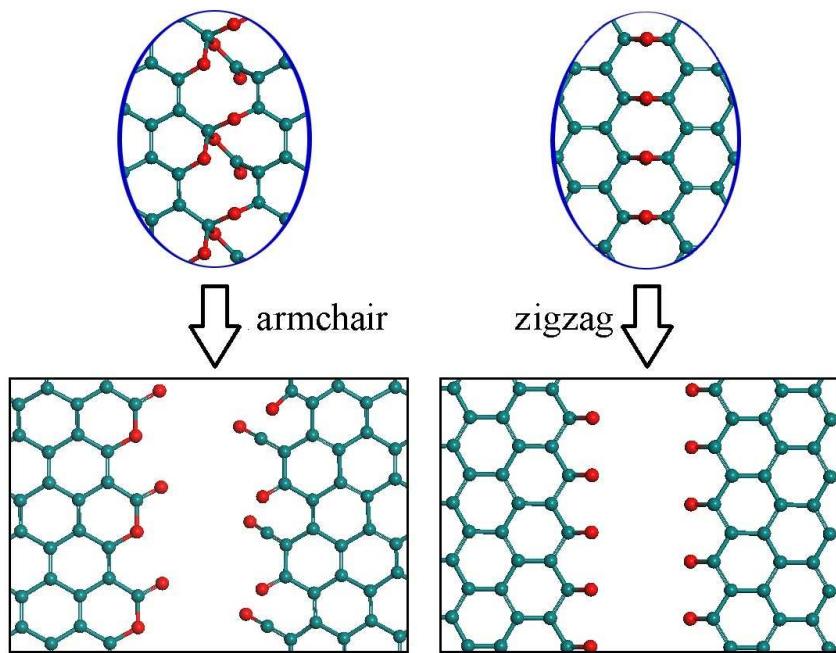


Fig. S3 Unzipping nanotubes along the armchair and zigzag directions in left and right panels, respectively.

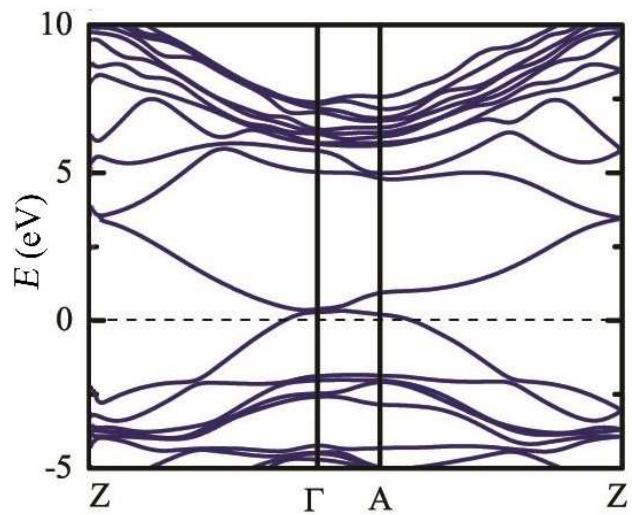


Fig. S4 Calculated band structure of epoxy-pair conformation using HSE06 functional.