Electronic Supplementary Information to

Controlling armchair and zigzag edges in oxidative cutting of graphene

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Binding energy calculations

Binding energy of first and nth O atom adsorption is calculated according to equations 1 and 2, respectively. The average binding energy of O atoms with pure graphene is calculated according to equation 3. The average binding energy of O atoms on strained graphene is also calculated according to equation 3; the only difference is that the total energy of pure graphene ($E_{graphene}$) and graphene-oxygen complexes ($E_{graphene + (n) oxygen}$) is calculated including strains (-5% to +5% with a increment of 1).

$$E_{BE}(1^{st}) = E_{graphene+oxygen} - E_{graphene} - E_{oxygen} \quad (1)$$

$$E_{BE}(n^{st}) = E_{graphene + (n) oxygen} - E_{graphene + (n-1) oxygen} - E_{oxygen} \quad (2)$$

$$E_{BE}(average) = [E_{graphene + (n) oxygen} - E_{graphene} - n^* E_{oxygen}]/n \quad (3)$$

Where, E_{BE} is the binding energy, $E_{graphene + (n) oxygen}$ is the total energy of graphene adsorbed with n O atoms, $E_{graphene}$ is the total energy of graphene, E_{oxygen} is the total energy of O atom.

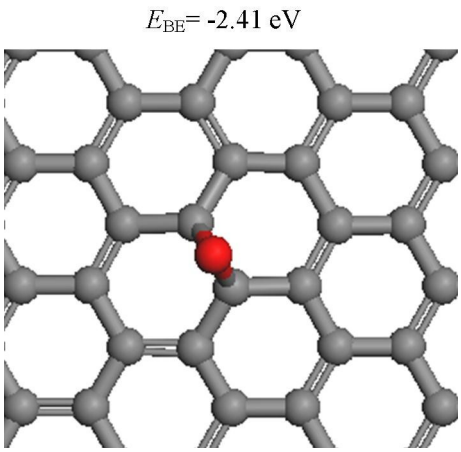

Fig. S1. Structure and binding energy (E_{BE}) of of oxidized graphene with one epoxy group.

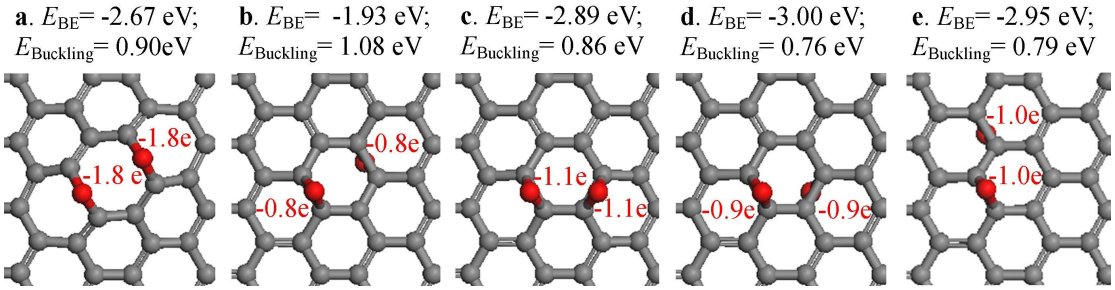

Fig. S2. Structure, binding energies (E_{BE}) and buckling energies ($E_{Buckling}$) of oxidized graphene with two epoxy groups. The red color text indicates the charge on O atom.

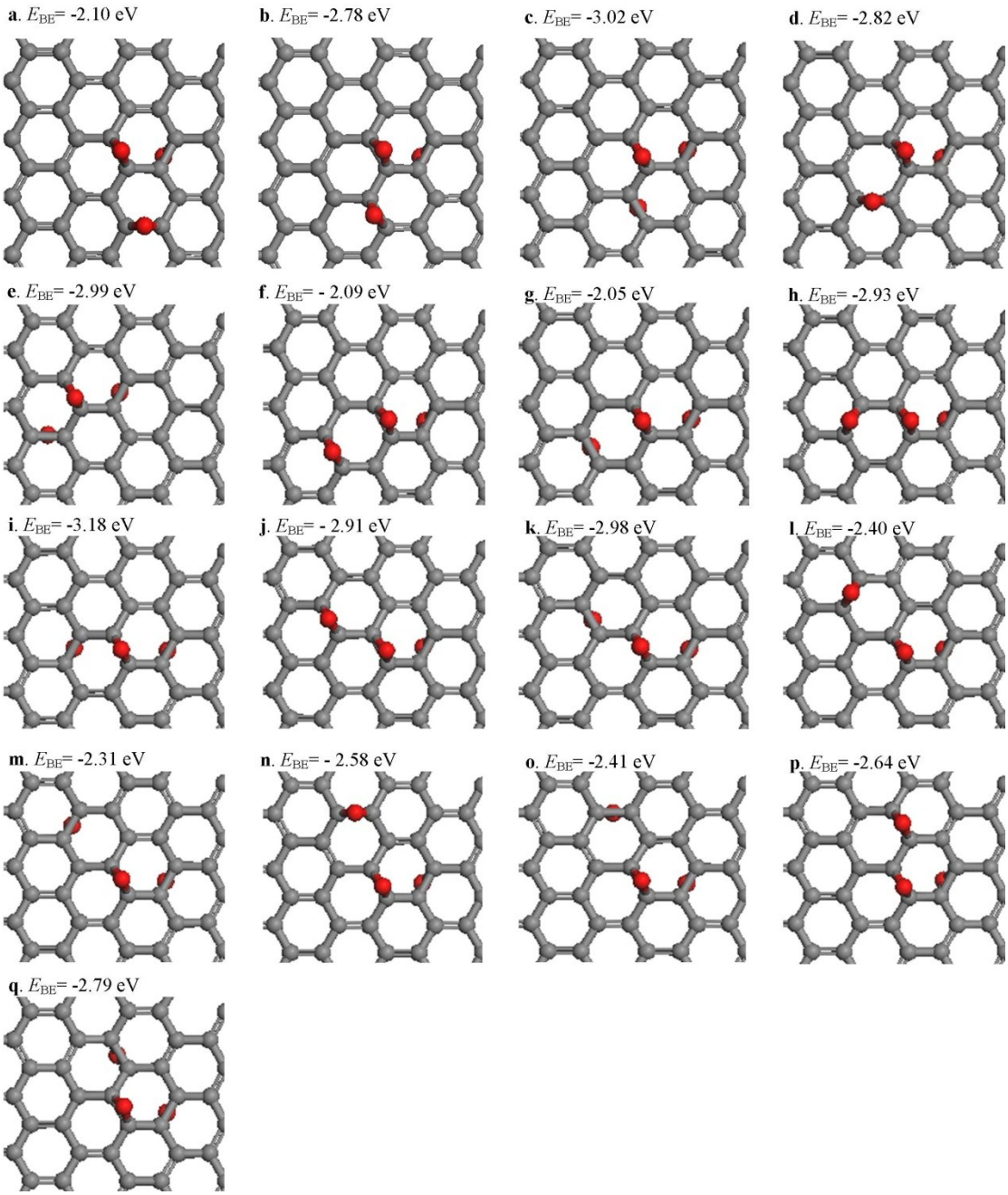

Fig. S3. Structure and binding energies (E_{BE}) of oxidized graphene with three epoxy groups.

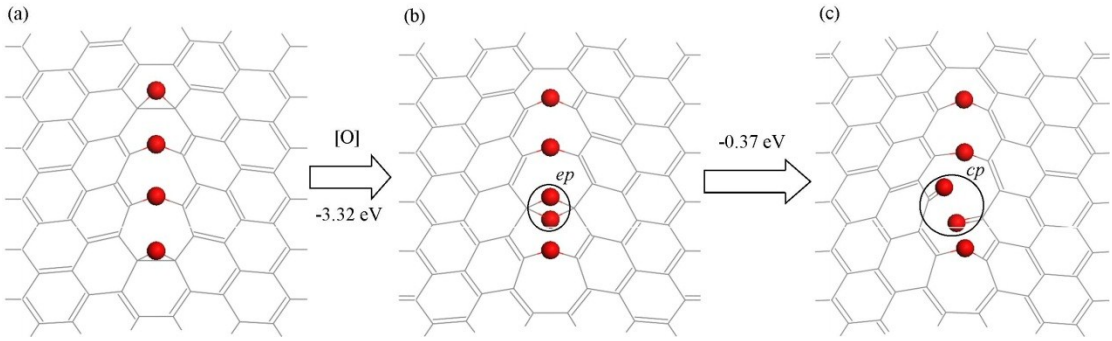

Fig. S4. Structure of oxidized graphene with (a) zigzag epoxy chain, (b) epoxy pair, ep and (c) carbonyl pair, cp.

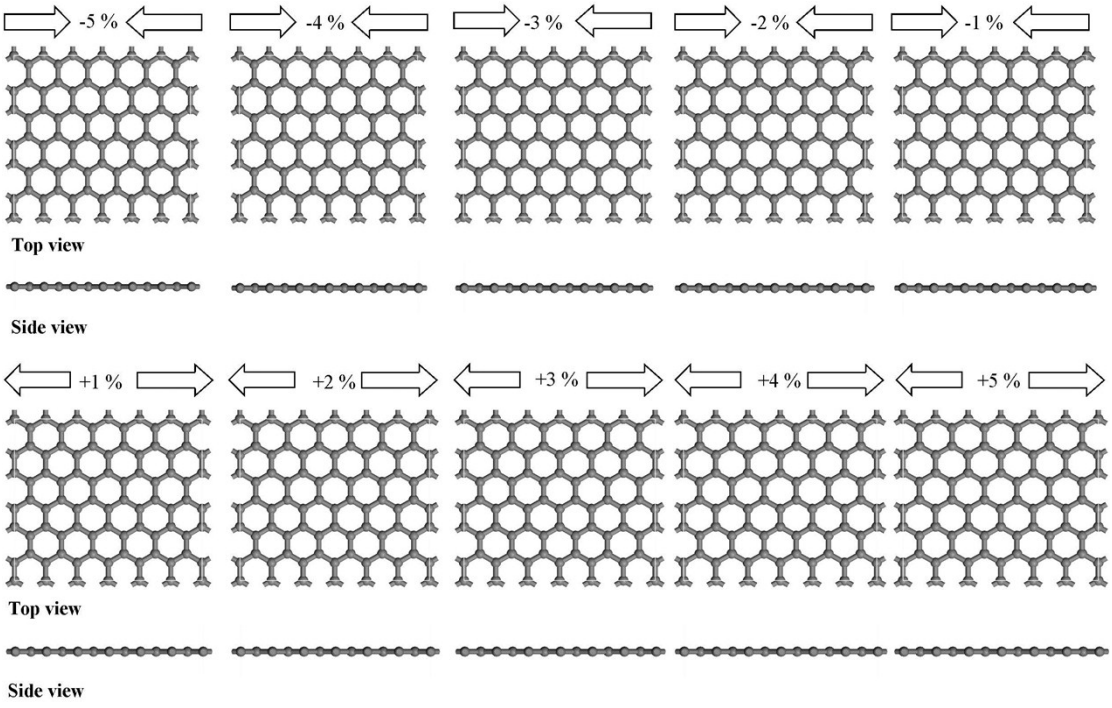

Fig. S5. Top view and side view of structure of graphene with strain (from -5% to +5%).

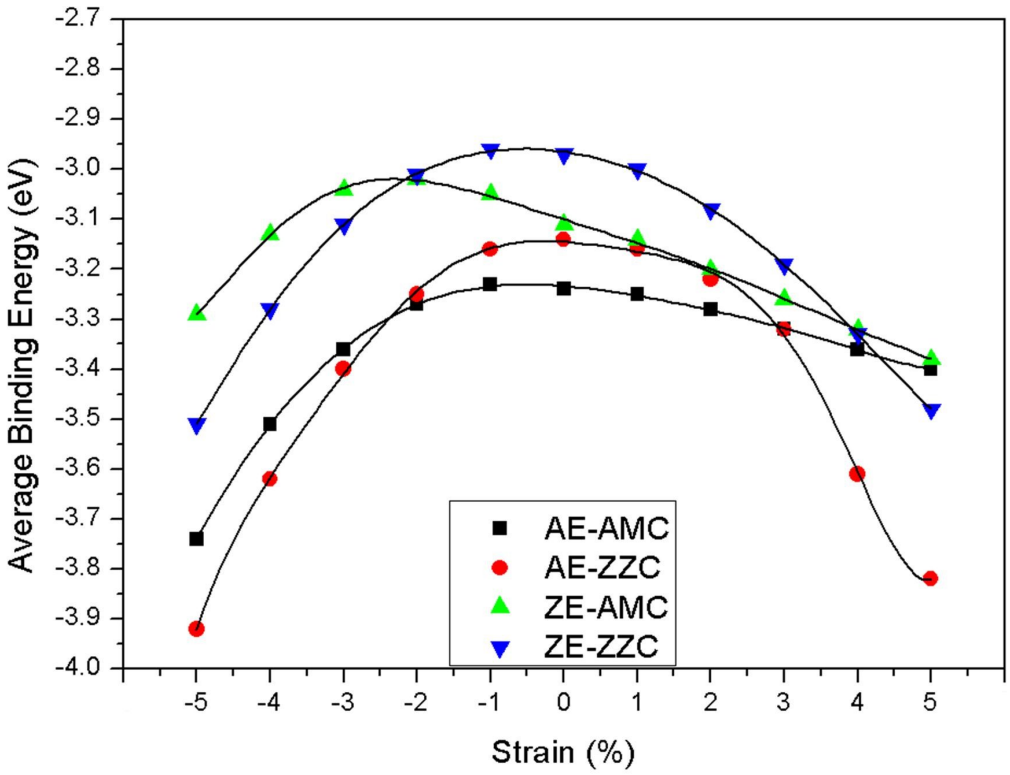

Fig. S6. Average binding energy of O atoms adsorption on graphene edge as a function of applied compressive and tensile strain. AE, ZE, AMC and ZZC indicate armchair edge zigzag edge, armchair epoxy chain and zigzag epoxy chain, respectively.