Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Electronic Supplementary Information (ESI)

# Chemical Bondings-Induced Rich Electronic Properties of Oxygen Adsorbed Few-layer Graphenes

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Table S1. The calculated adsorption energy, binding energy, O-O interaction energy and energy gap of GO with various oxygen concentrations.

| O Concentration | Adsorption energy (eV) | Binding energy (eV) | O-O interaction energy (eV) | Energy gap (eV) |
|---|---|---|---|---|
| 50% (single-side, zigzag) | -2.9390 | -4.4651 | 1.5262 | 3.54 |
| 50% (single-side, armchair) | -2.4258 | -4.0943 | 1.6686 | 2.83 |
| 50% (single-side, chiral) | -2.6052 | -4.2957 | 1.6905 | 3.92 |
| 33.3% (single-side, armchair) | -2.3728 | -3.7433 | 1.3705 | 2.53 |
| 25% (single-side, zigzag) | -2.3515 | -3.6509 | 1.2995 | 0.63 |
| 50% (both-side, zigzag) | -4.4079 | -4.8622 | 0.4543 | 3.14 |
| 33.3% (both-side, armchair) | -4.3919 | -4.6682 | 0.2763 | 2.47 |
| 25% both-side, zigzag) | -4.2676 | -4.5079 | 0.2403 | 0.17 |

The adsorption energy is defined as

$$E_{ad} = (E_{sys} - E_{gra} - E_{oxy})/n \tag{1}$$

where $E_{sys}$, $E_{gra}$, and $E_{oxy}$ are the total energies of the GO system, the graphene sheet, and the oxygen cluster of n atoms, respectively.

The binding energy is defined as

$$E_b = (E_{sys} - E_{gra} - nE_O)/n \tag{2}$$

where $E_O$ is the total energy of an isolated O atom.

The O-O interaction is characterized by the energy difference between $E_{ad}$ and $E_b$.

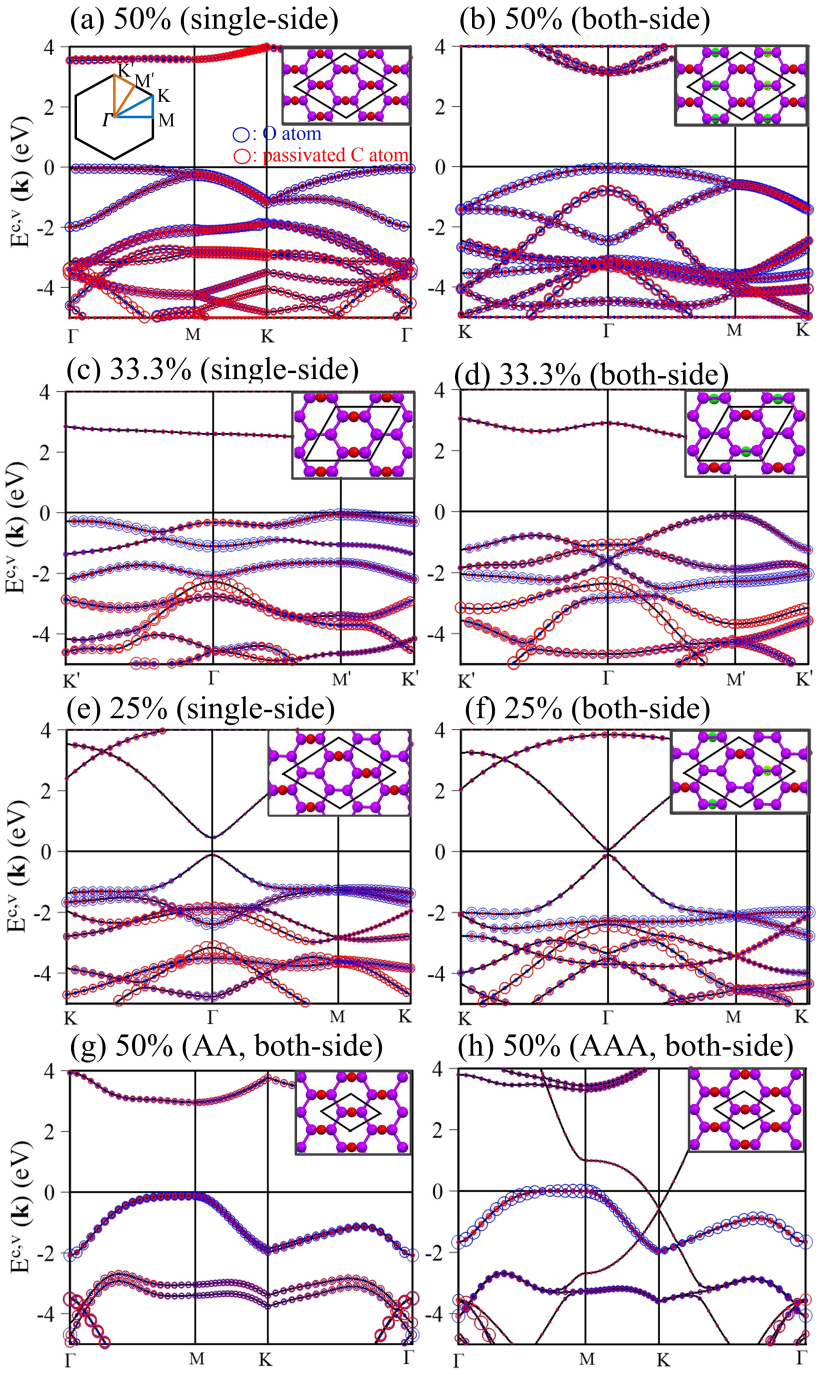


Figure S1. Band structures of GO with the oxygen concentration of: (a) 50% (single-side), (b) 50% (both-side), (c) 33.3% (single-side), (d) 33.3% (both-side), (e) 25% (single-side), (f) 25% (both-side), (g) 50% (AA, both-side), and (h) 50% (AAA, both-side). The red and green atoms represent the top- and bottom-adsorption of O atoms on graphenes, respectively.

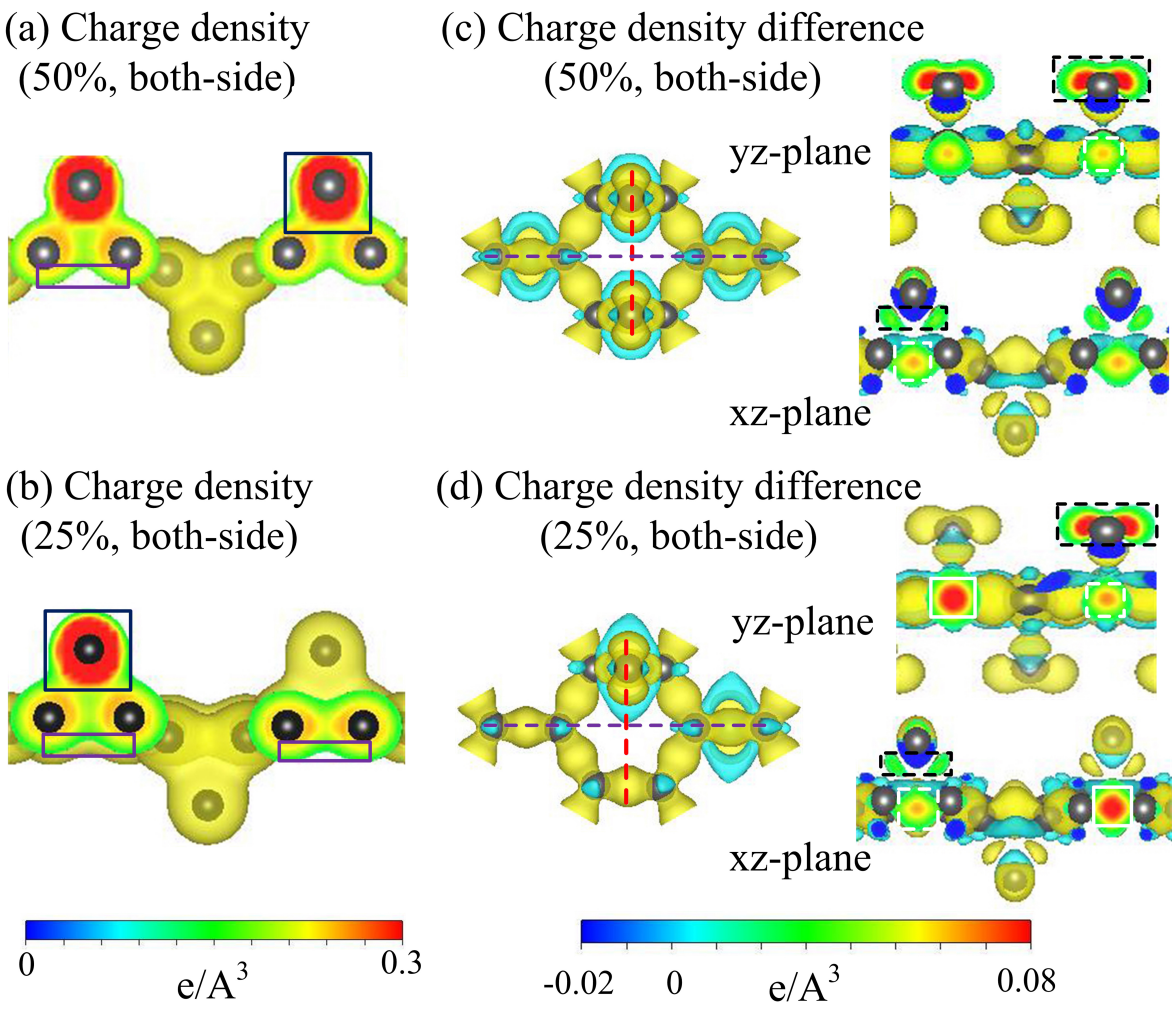


Figure S2. The charge density of (a) 50% (both-side), and (b) 25% (both-side). The charge density difference in yz- and xz-planes of (c) 50% (both-side), and (d) 25% (both-side).