CAPACITIVE PROPERTIES OF GRAPHENE WITH INCORPORATED COBALT OXIDE PARTICLES

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The aim of the work to theoretically find out the regularities of Co3O4 nanocubes binding to the surface of pure graphene, graphene with substitutional oxygen and graphene oxide with the following obtaining of Co3O4/rGO nanocomposite by the self-consistent charge density functional tight-binding (SCC DFTB) method. The most favorable hybrid materials for lightweight SCs will be found from the view of energetic and capacitive parameters.

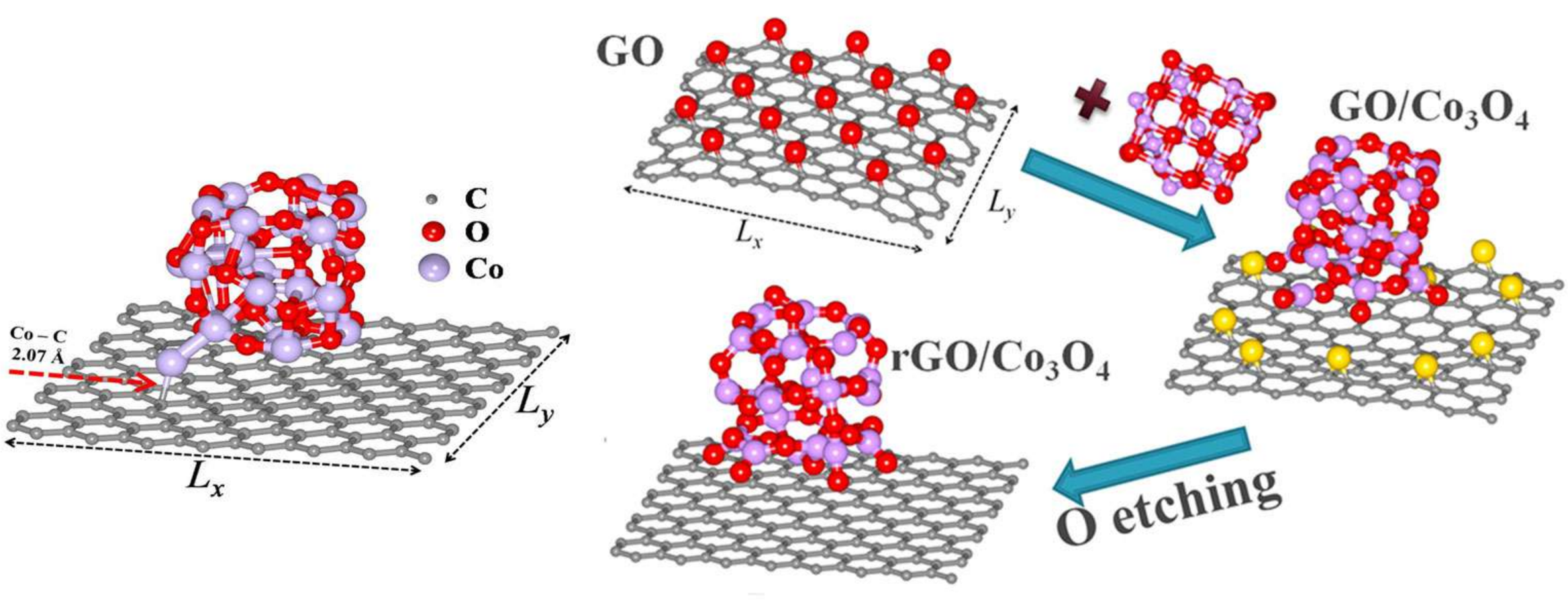
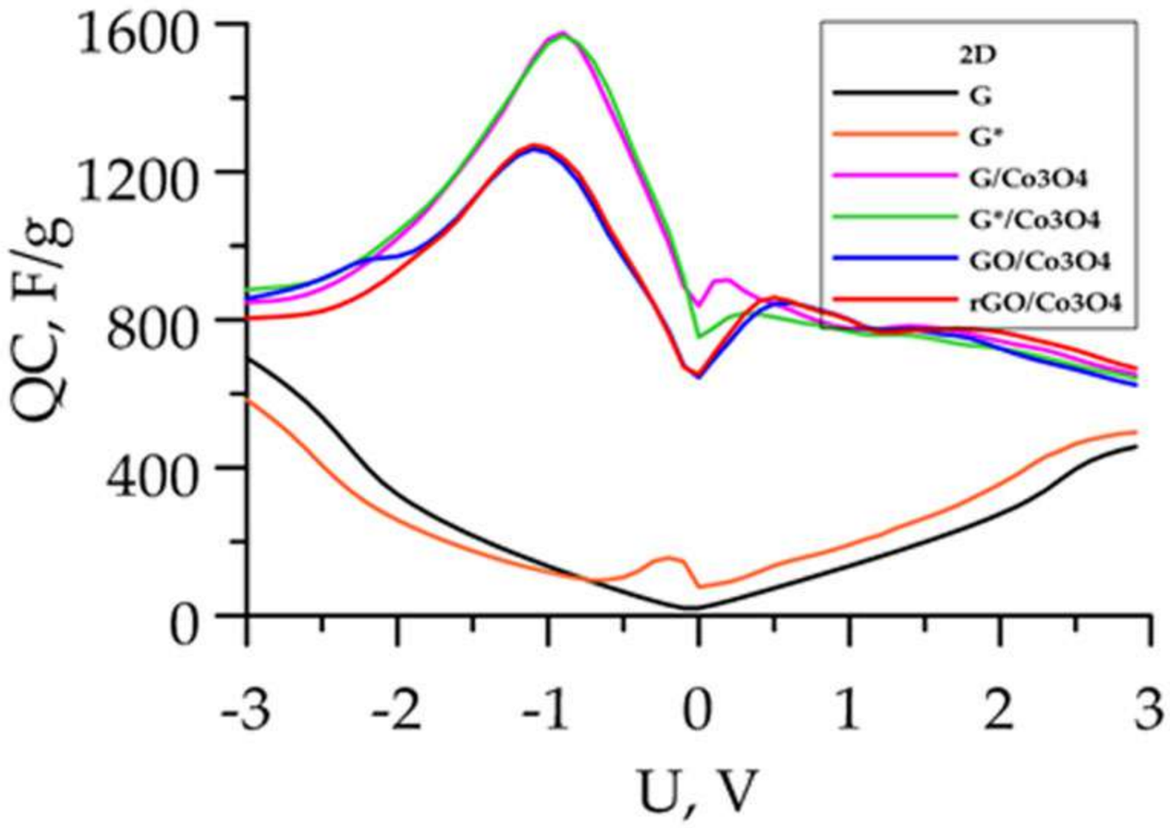


Figure 1. The atomic structure of (a) the G/Co3O4 nanocomposite; (b) the G*/Co3O4 nanocomposite. The translation vectors are Lx = 19.78 Å and Ly = 21.41 Å.The atomic supercell of the membranes G/Fe3O4 after optimization by the method SCC DFTB with mass ratios: a) 1:1 top view; b) 1:1 side view with translation vectors Lx and Ly;

Table 1.Fermi level, charge transfer and value of QC at the U=0V for pure graphene and 2D-composites: G/Co3O4, GO/Co3O4, rGO/Co3O4.

	Fermi level, eV	**Charge, e**	**QC(0V), F/g**
G	–4.67		20.78
2D G/Co_3O_4	–3.50	1.15	837.55
2D GO/Co_3O_4	–3.57	1.38	644.25
2D rGO/Co_3O_4	–3.48	0.88	652.17



Conclusion:

The attempt to compare adhesion and electronic properties of G/Co3O4 and rGO/Co3O4 nanocomposites was performed for the first time by the SCC DFTB method. Our calculation showed that the formation of the rGO/Co3O4 started from attachment of Co3O4 nanocubes to GO surface with consequent etching of oxygen atoms is more favorable than the straight decoration of G with Co3O4 nanoparticles both for 2D-films. The addition of Co3O4 nanoparticles to G shifts Fermi level to 1.10÷1.41 eV that indicates the enhancement of conductive properties. The dependence of QC on voltage showed the significant improvement of capacitance in the case of G in comparison to rGO. In dependence of applied voltage this difference varies in the range of 300÷500 F/g. In the Introduction it was mentioned that G/Co3O4 are obtained from GO that leads to retention of oxygen atoms and to decrease in total capacitance. So one of the main challenges in this field is connected with straight synthesis of G/Co3O4 from pure G.

Shunaev V.V., Glukhova O.E. Interaction of Co3O4 Nanocube with Graphene and Reduced Graphene Oxide: Adhesion and Quantum Capacitance. Lubricants. 2022; 10(5):79.