Functionalized Graphene Bio-Sensing Building-Blocks under Environmental Stimuli

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Introduction: This study continues to investigate the main properties of graphene (G/RGO/GO), and other C allotrope nanostructures for biosensors design, using COMSOL Multiphysics® modules.

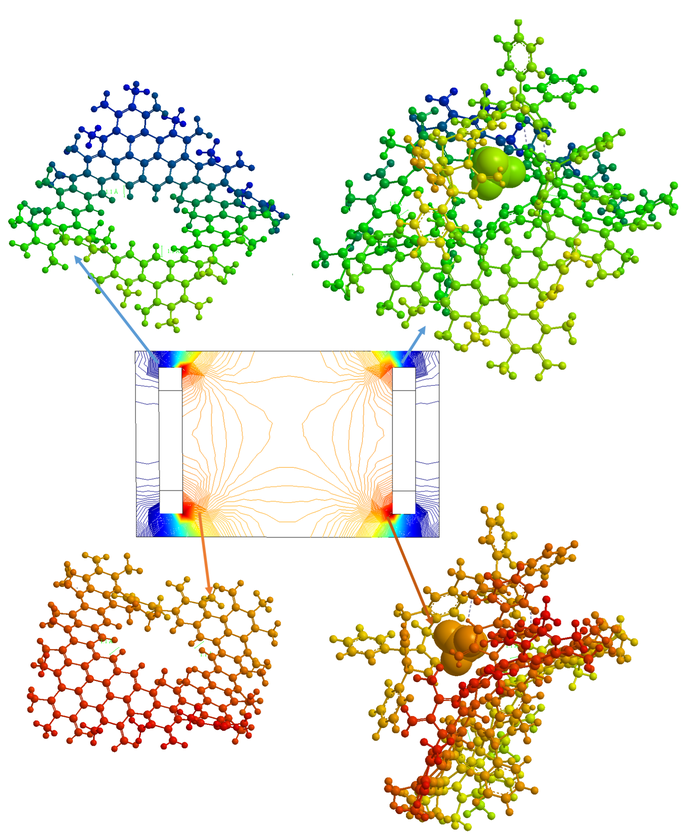

Figure 1. Functionalized G/GO/RGO bio-sensing modules

Computational Methods: Electrical Potential Profile is a function of distance (x) from graphene surface. The shape of potential function is determined by Modified Poisson-Boltzmann equation (Eq.1):

$$\frac{d^2V}{dx^2}=\sum_i \frac{z_i e c_{0i}}{\varepsilon}\cdot\frac{2\sinh\left(\frac{z_i eV}{kT}\right)}{1+2v_i sinh^2\left(\frac{z_i eV}{2kT}\right)} \qquad (1)$$

In MATLAB code (P- potential, used instead V from Eq.1) all simulation parameters are (Eq.2): $[x,P,R]=potential\_1D(P\_0,Z_i,C_i,E\_R,EFF,MPB)$
One of the simulation output parameters is ion concentration as a function of the distance from graphene surface (Eq.3):

$$C_i=C_{i0}e^{\frac{-z_i eV(x)}{kT}} \qquad (3)$$

MATLAB application of graphene properties (Fig.2a,b,c) and CNTs (Fig.2c) in specific models and simulations were exported through LiveLink in COMSOL Multiphysics® (Fig.3c,4c,5b).

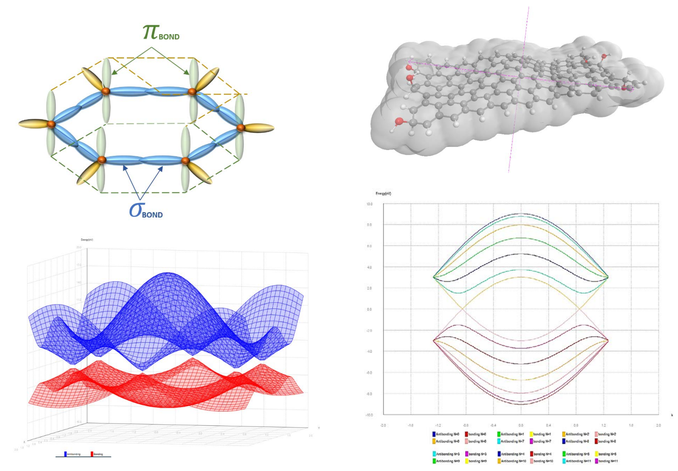

Figure 2. Carbon allotropes studies
(a) G unit cell; (b)G -T.Char.Density;
(b) MATLAB computed properties (c) G (10,10); (d) CNT (6,6,10)

Results: With COMSOL Multiphysics® modules, importing geometry and properties from ChemBio3D on Electrochemistry module, and the electrical and the thermal properties from MATLAB through LiveLinkTM on Multiphysics were performed different functionalization simulations (Fig. 3-5)

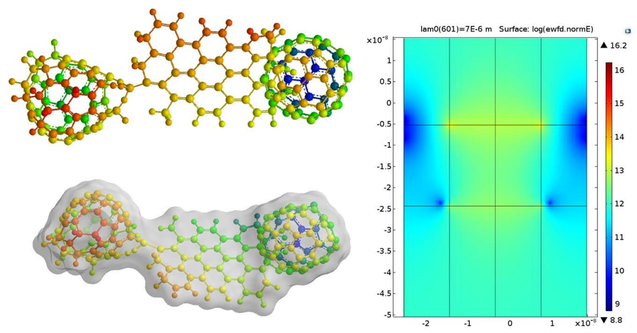

Figure 3. RGO- 2xC60 self-assembly :
(a) model ; (b) Total Charge Density ; (c) Electrical Potential Profile

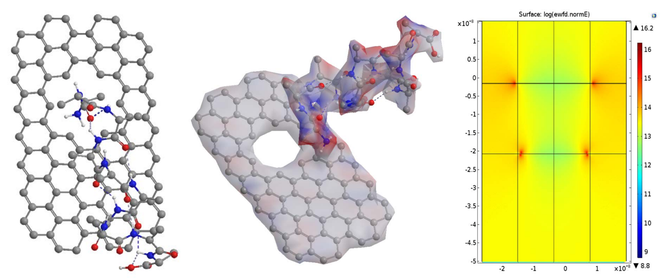

Figure 4. GO- Alpha-Helix (protein) self-assembly :
(a) model ; (b) Total Charge Density ; (c) Electrical Potential Profile

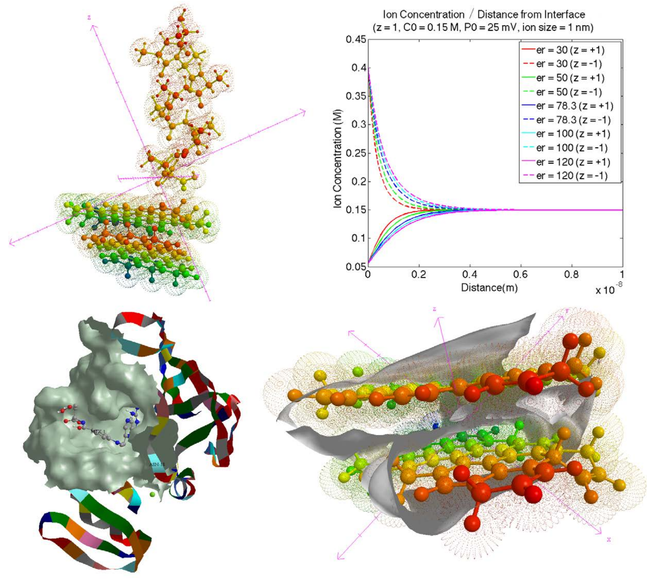

Figure 5. 2x RGO(1-pore)- Alpha-Helix- self-assembly :
(a) Self-Assembly model ; (b) Ion concentration;
(b) (c) Local Charge Density – Protein-RGO pore ;
(c) (d) 2xRGO –Total Charge Density