

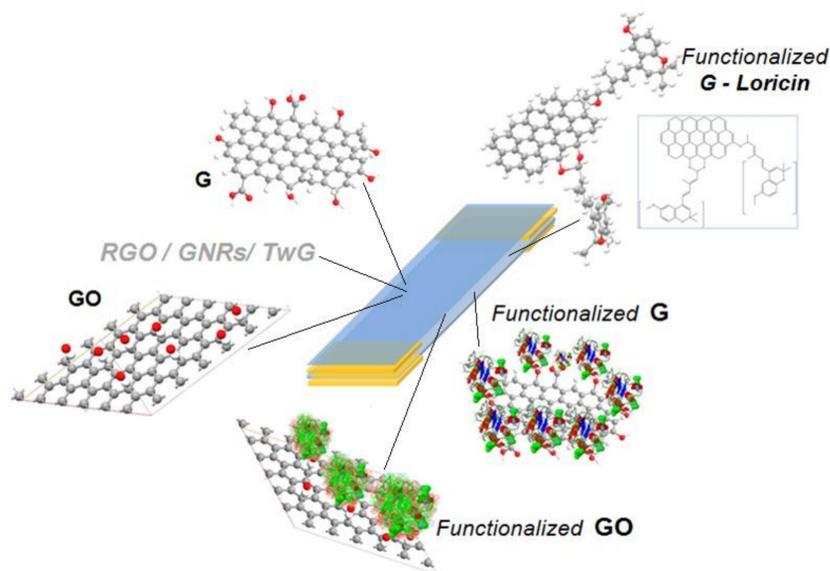
# Models for Simulation Based Selection of 3D Multilayered Graphene Biosensors

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**Introduction:** Through COMSOL Multiphysics modeling and simulation were identified the best fitted solutions for a multilayered biosensing device structure from the presently known graphene (and composite materials including different forms of graphene).

**Results:** A large number of device module types have been tested in order to define the best response of the hydrogel- polymer layer (PVA Hydrogel) on the graphene sheets and of the protein functionalized graphene biosensors.



**Figure 1.** Basic and functionalized graphene structure models (ChemBio 3D Ultra<sup>®</sup>)

**Computational Methods:** All these models are having the same continuum-like background of a biosensor device structure based on weak van der Waals interaction forces that describe the nonlinear behavior of graphene into a surrounding viscoelastic environment through classical Kirchhoff plate theory

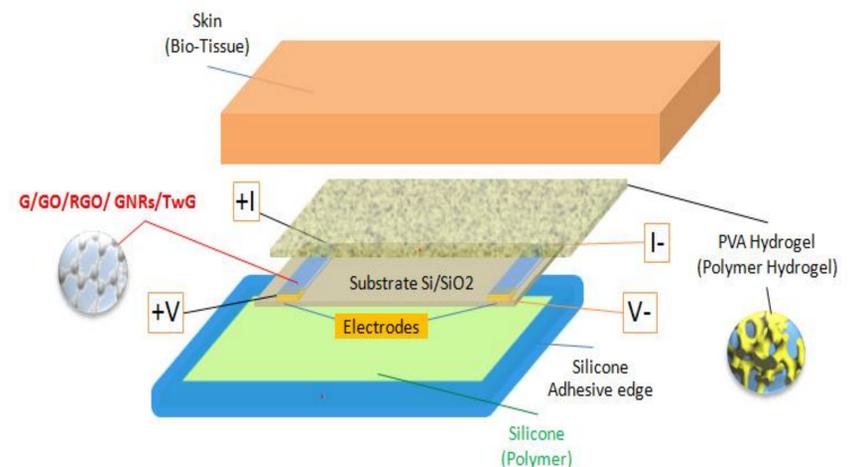
$$D\nabla^4 w + \alpha_1 w + \alpha_3 w^3 + \rho h \frac{\partial^2 w}{\partial t^2} + N_x \frac{\partial^2 w}{\partial x^2} + N_y \frac{\partial^2 w}{\partial y^2} = 0 \quad (1)$$

where:  $N_x$ ,  $N_y$  are biaxial in-plane loads;  $a$ ,  $b$ - length, width of graphene;  $h$ - thickness of graphene;  $p$  – distributed transverse load per unit area (due to surrounding medium effect) ;  $D$  is the bending stiffness of the plate:

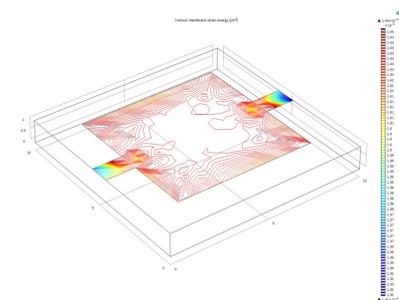
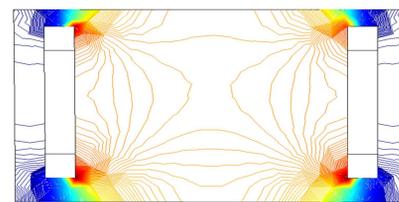
$$D = \frac{Eh^3}{12(1-\nu^2)} \quad (2)$$

for all models were studied the charge density distributions of electric, thermal and acoustic field stimuli responsible for ( $\bar{e} - ph$ ), ( $ph - ph$ ) and ( $ion - ph$ ) interactions.

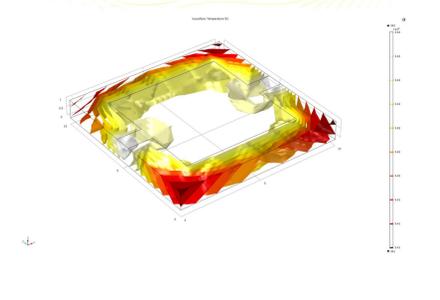
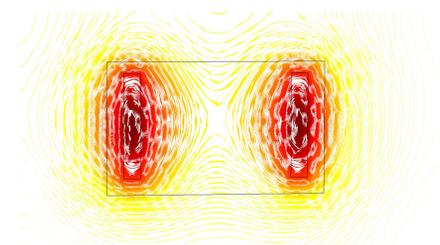
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**Figure 3.** Multilayer graphene sensing device



**Figure 4.** Electric potential  
(a) 2 electrodes device; (b) 4 electrodes device



**Figure 5.** Temperature  
(a) 2 electrodes device; (b) 4 electrodes device

**Conclusions:** For each module type the graphene/ graphene composite materials generate clearly differentiate responses to the environmental stimuli, or process microvariables evolution, thus confirming the biosensing ability of this class of materials.

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