COMSOL Multiphysics® Simulation of Functionalized 3D Biocompatible Porous Graphene Composites

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Introduction:
Being alike an indefinitely large aromatic molecule, graphene has exceptional mechanical, electrical and thermal properties. Moreover, being one-layer thick is almost transparent (fig.1), thus interacting with light and with other materials in unprecedented ways within functionalized graphene embedded composites (fig.1-5)

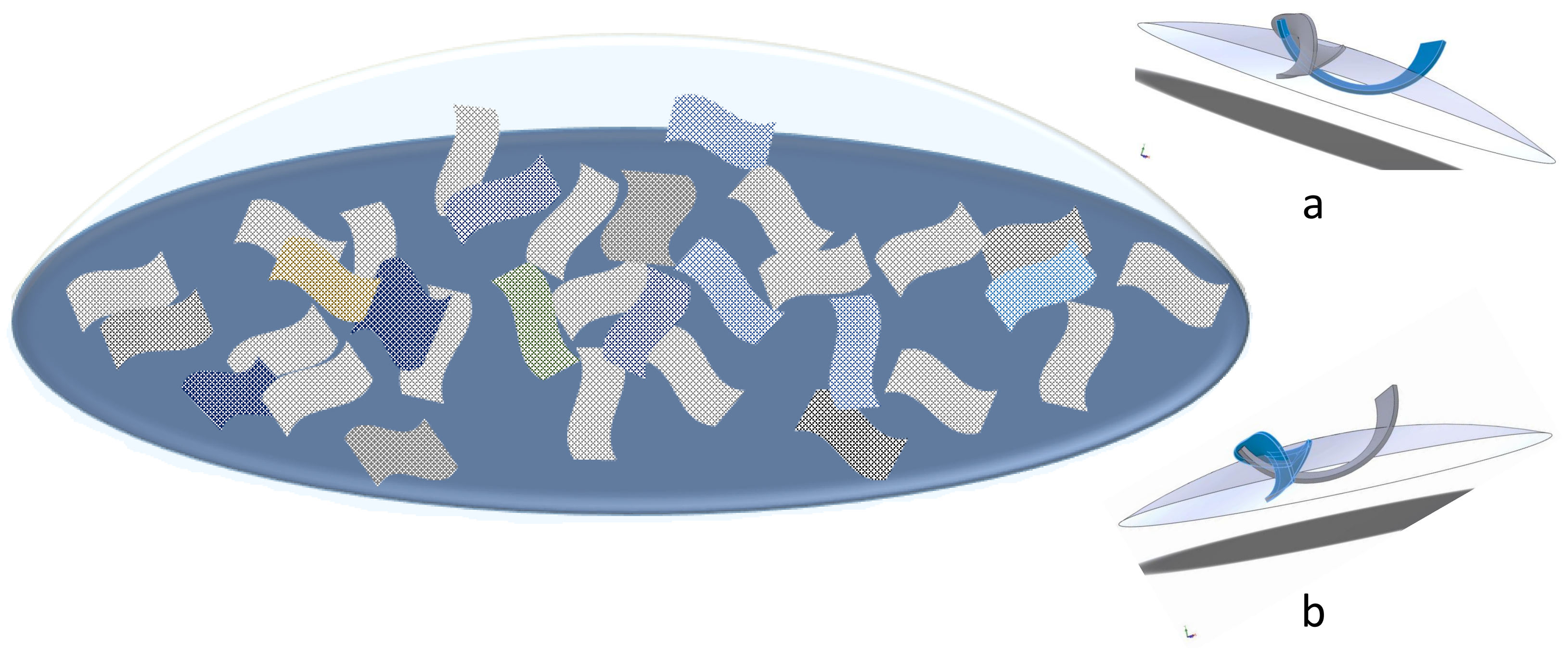

Figure 1. Individual graphene (G/GO) composite cell
(a,b) Porous support with randomly disposed twisted (G/Go) layers

Computational Methods:

G/GO related physics was introduced in COMSOL Multiphysics® through the bidirectional interface with MATLAB® via LiveLinkTM for MATLAB . While the geometry of G/GO and of the biosensor parts were exported as SolidWorks® models through LiveLink™ for SolidWorks® add-on in COMSOL Multiphysics®

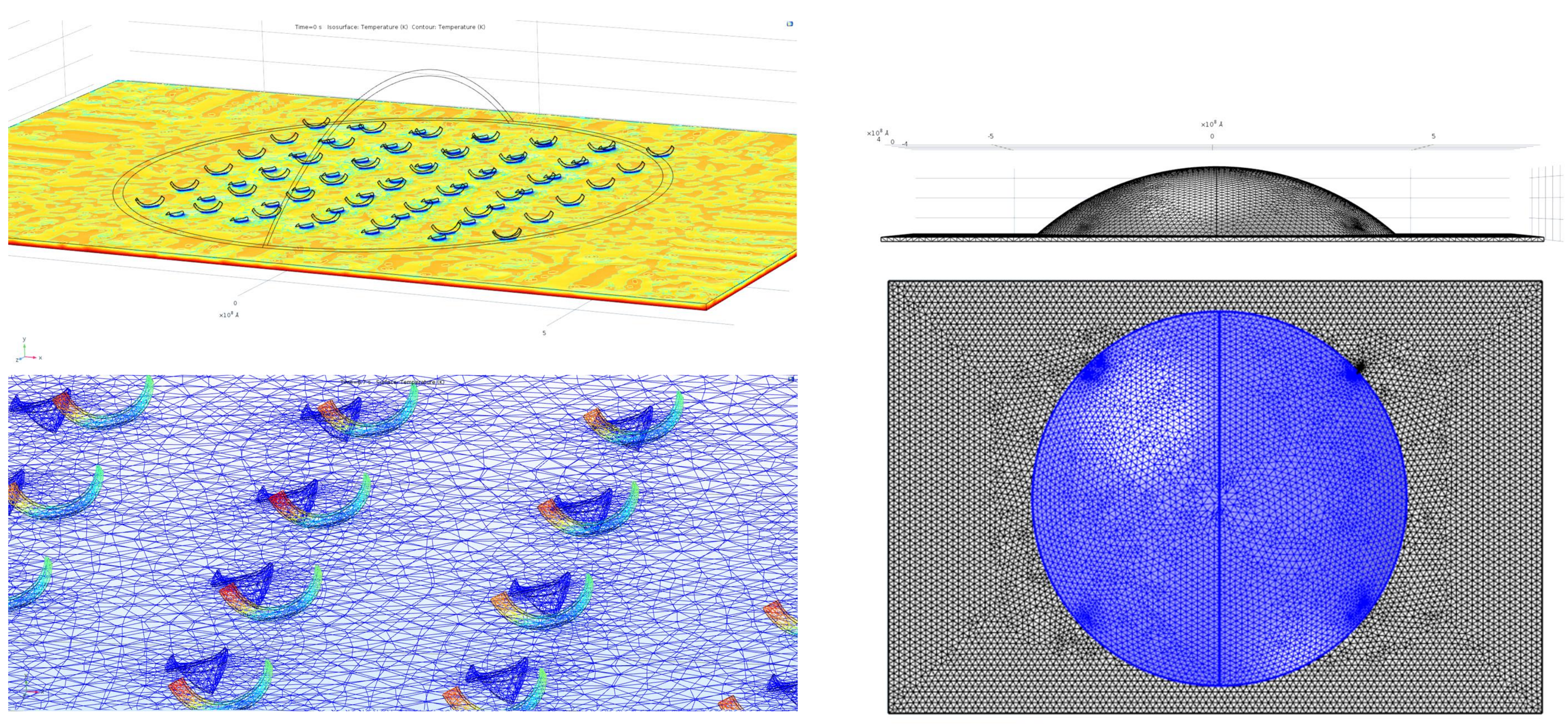

Figure 2. Physical model of biocompatible (G/GO) composite cell
a. Successive layers and shells containing (G/GO) structures
(b, c) Mesh of graphene embedded structures

Results:
The results of the COMSOL Multiphysics® simulations for functionalized 3D biocompatible porous G/GO composites (fig.3-5) were validated using SoA literature data related to photodermal therapy (PTT), photodynamic therapy (PDT) and drug delivery through skin processes and parameters.

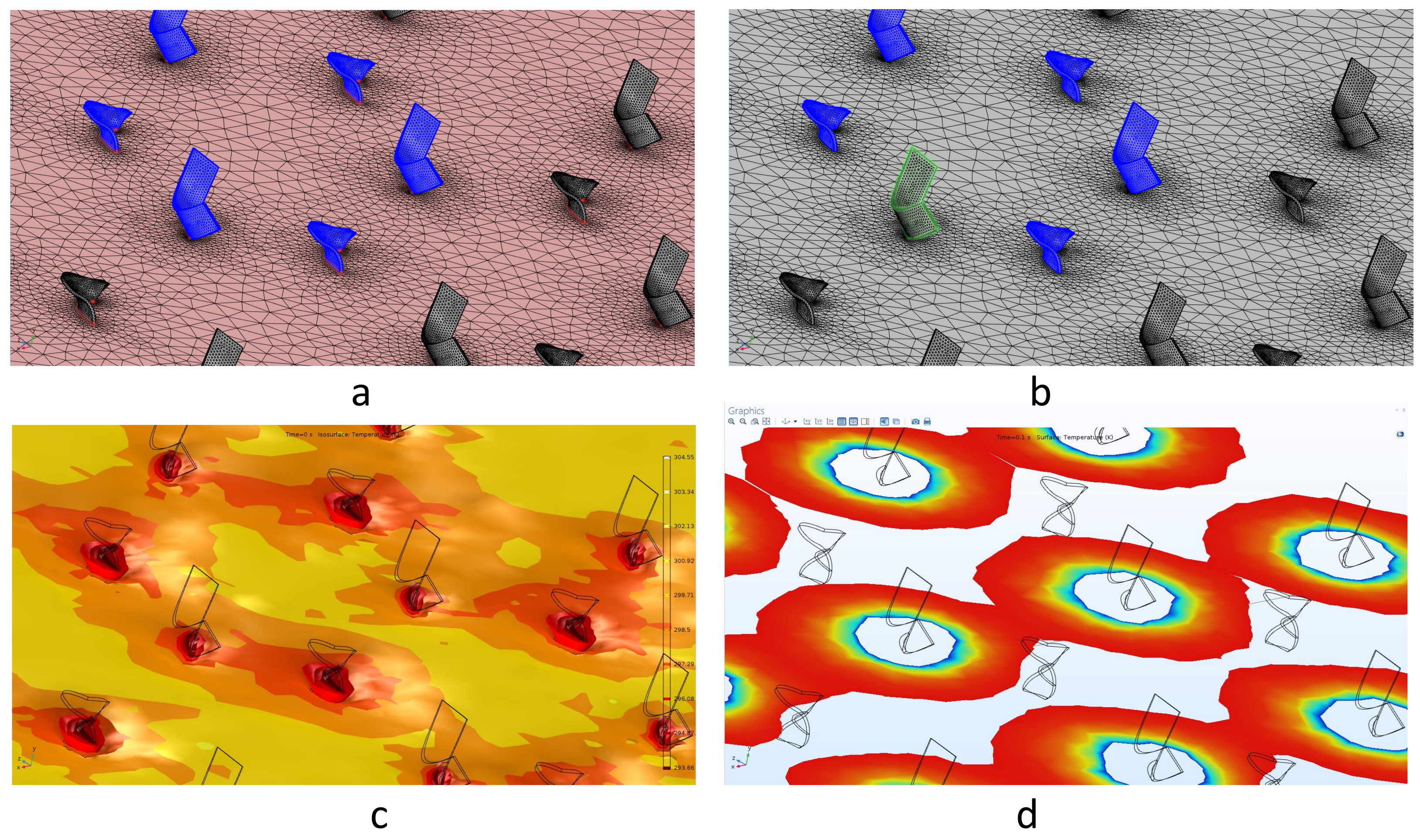

Figure 3. Response of the excited G/GO – composite
(a) Array excitation – global response (c) ;
(b) Individual excitation- Singularities response (d)

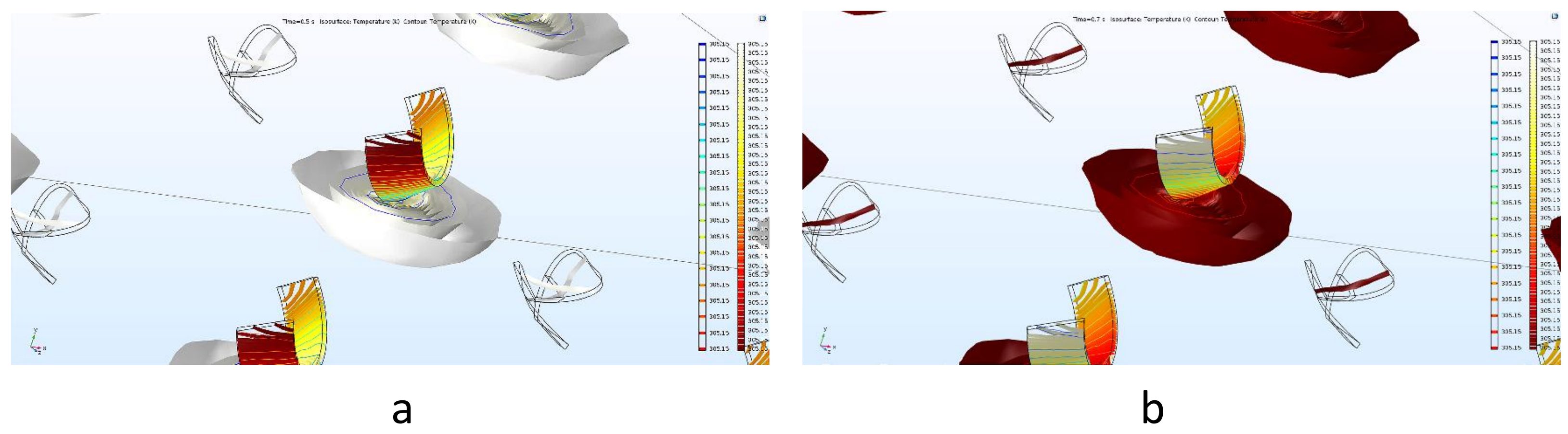

Figure 4. G/GO shape and position influence biosensor response to environmental stimuli (a,b)

Conclusions:
Material properties for G/GO were added to Material Library dBs. The use of COMSOL Multiphysics® was focused on heat transfer modules (shells, films, porous media, bioheat) but as well on the use of Schrödinger Equations for the very particular properties of G/GO structures.

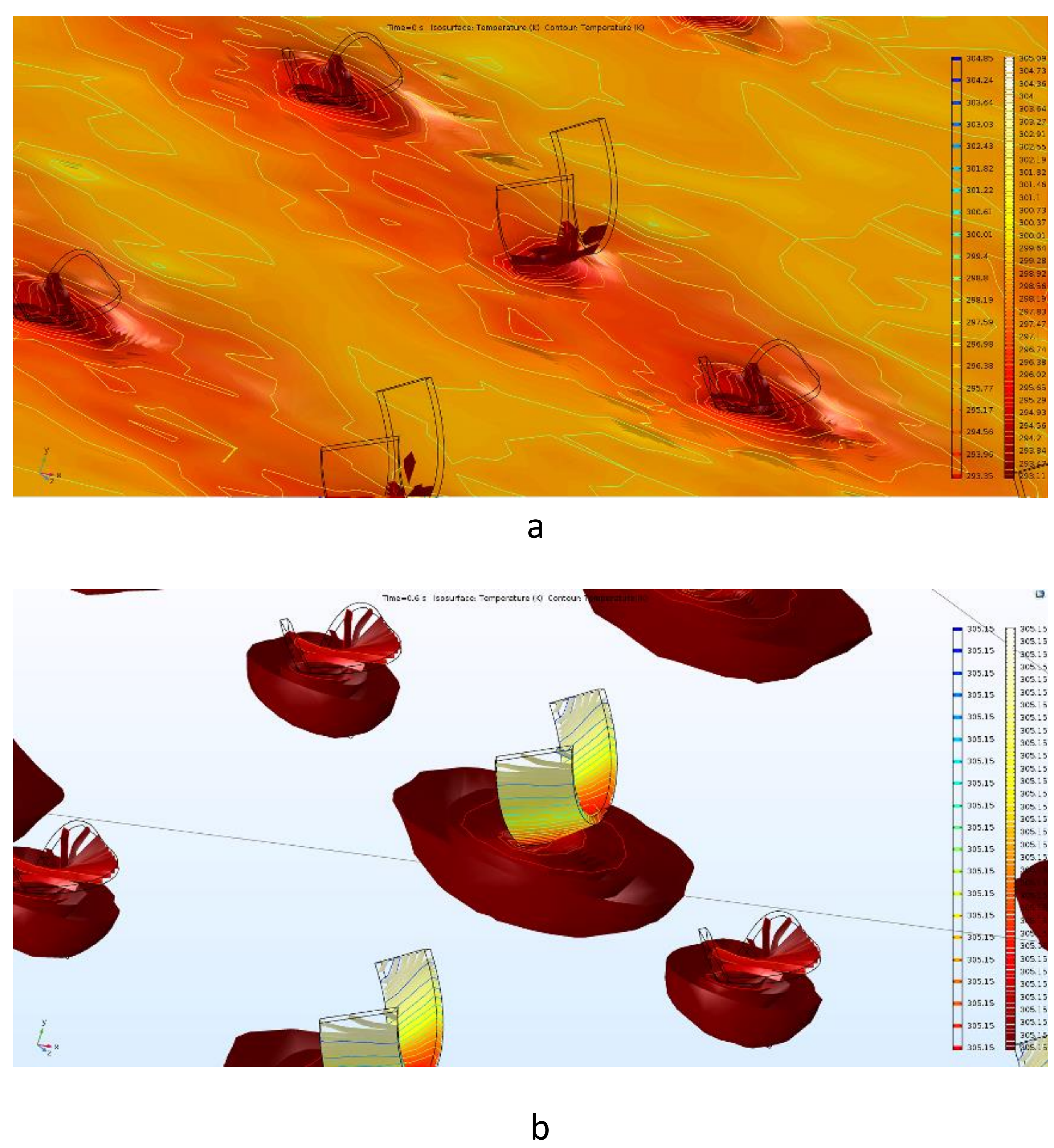

Figure 5. Differentiated time response of excited G/GO structures to simulation data

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