**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 LiveLink™ 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