

Introduction: Bio-compatible G/GO/RGO composite structures with embedded stearic acid on a bilayer structure model, biomimicking the cellular lipid bilayer are introduced through successive models.

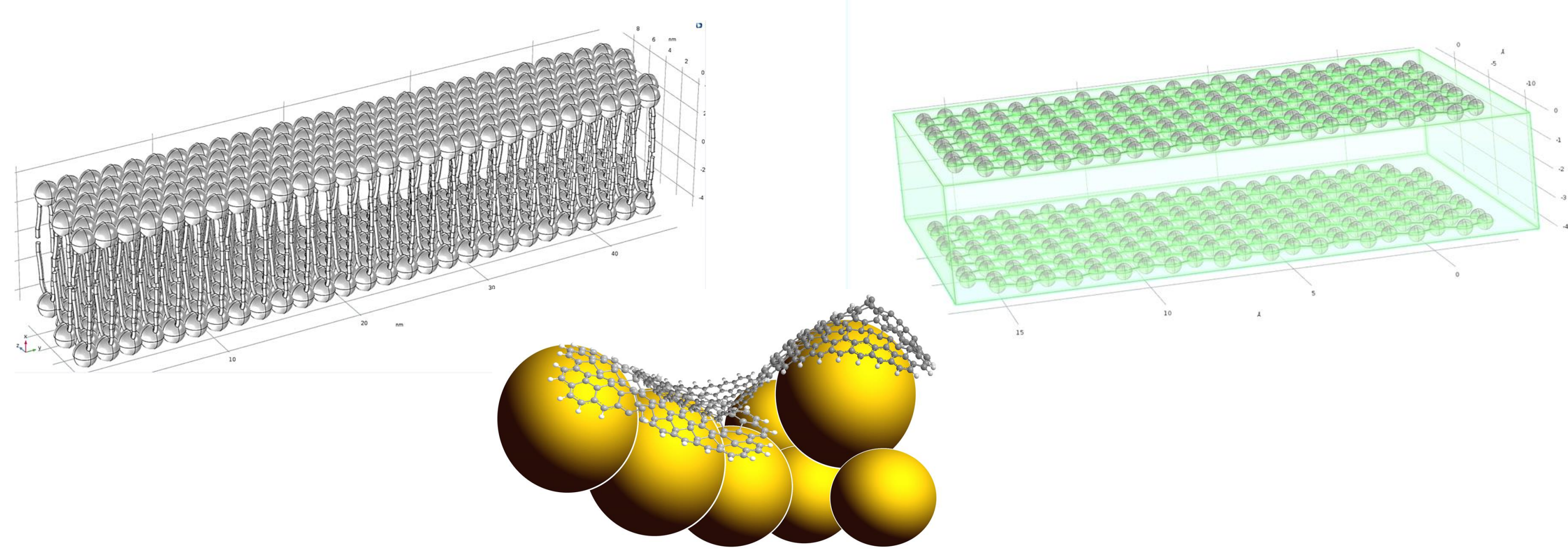


Figure 1. Graphene vs. Lipid Bilayer

Computational Methods: The solvent accessible surface of the models (van der Waals surface) and the related MD values were imported from Molecular Dynamics through MATLAB® studies, using LiveLink™ for MATLAB®. Within the modeling, simulation and validation of the graphene-assisted-lipid bilayer were used as well: COMSOL Multiphysics®, CFD, Semiconductor and Particle Tracing modules.

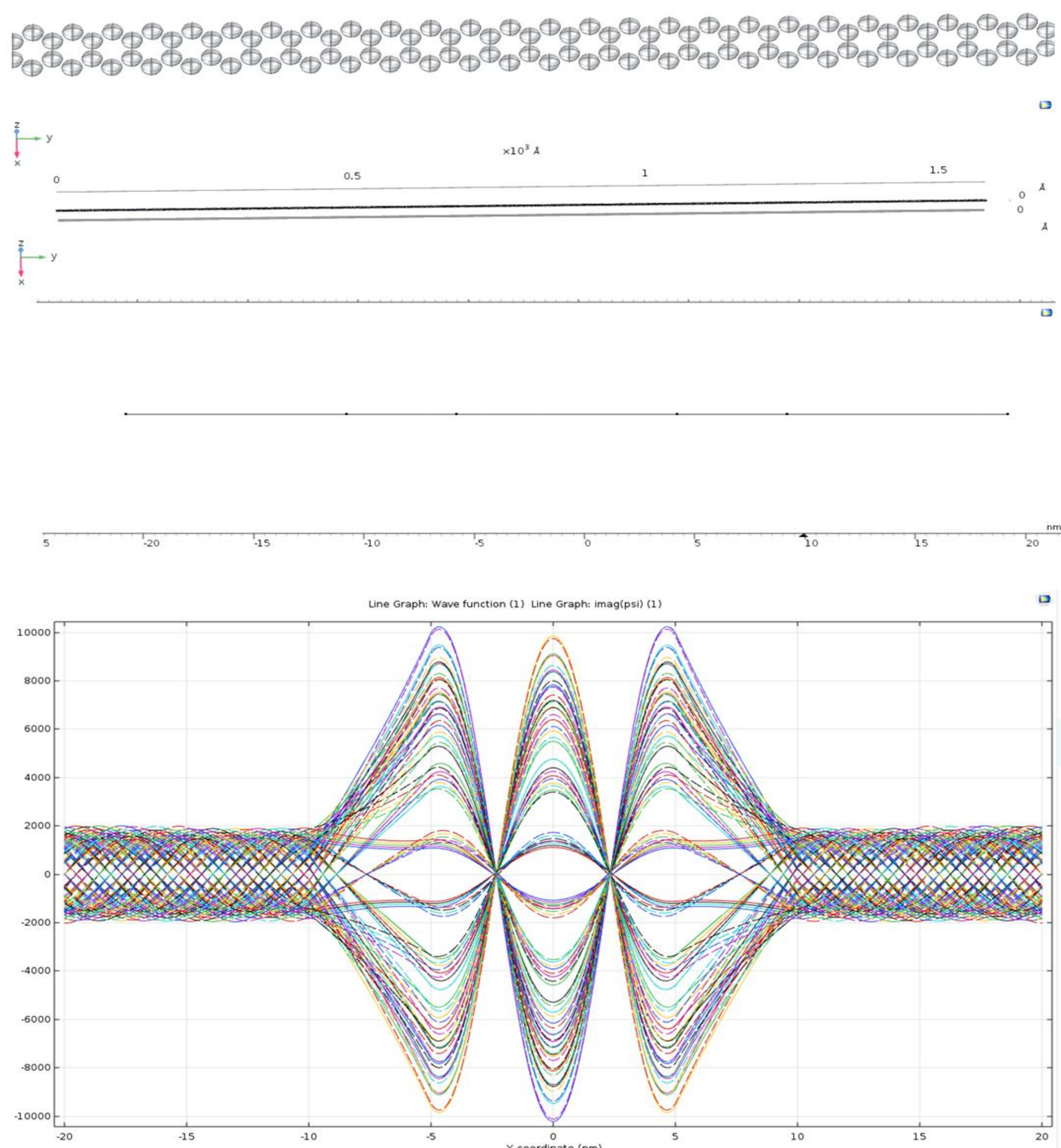


Figure 2. Graphene Ribbon -1D model of Cell Membrane (successive models at real size)

Results:

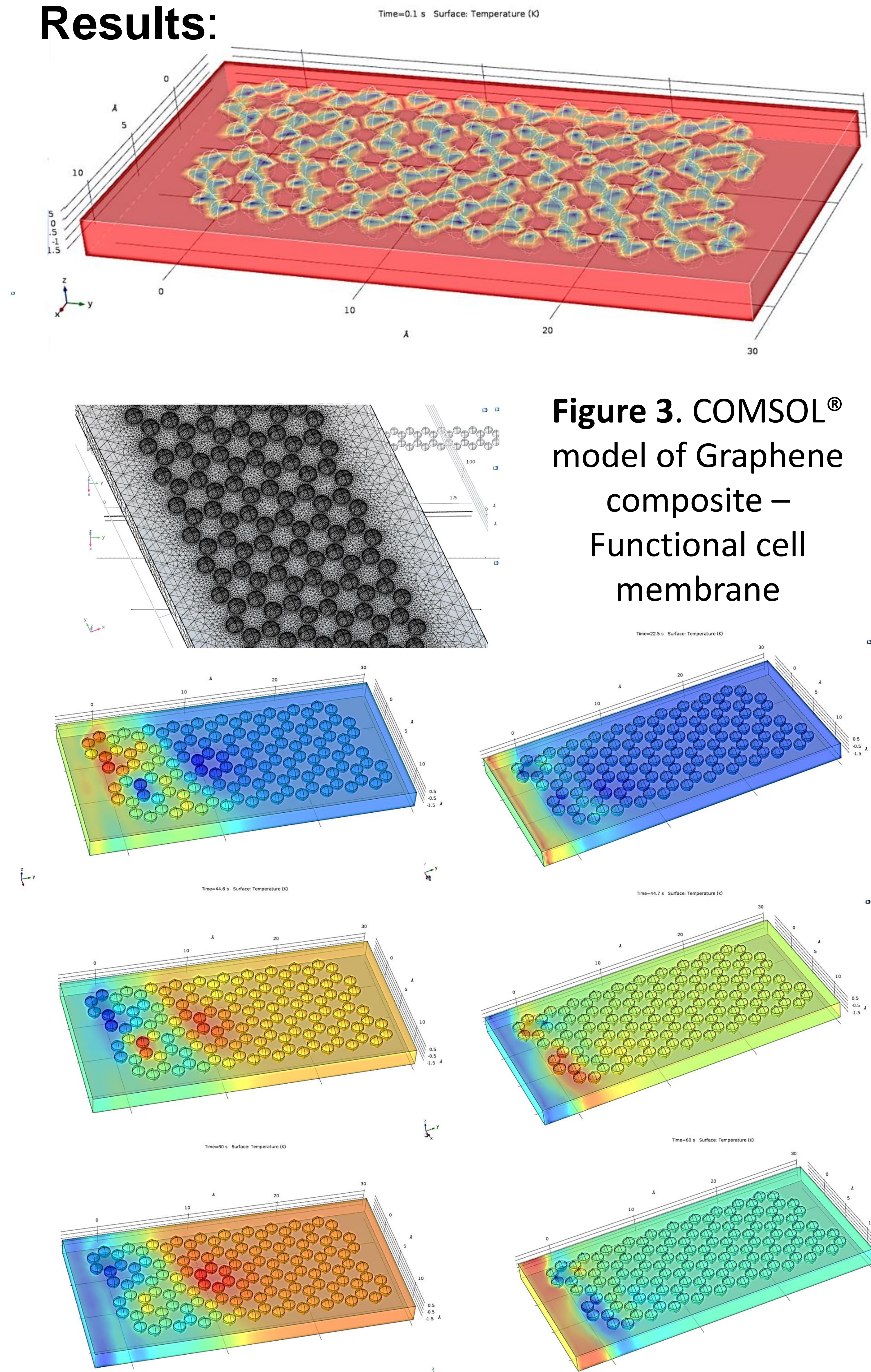


Figure 3. COMSOL® model of Graphene composite – Functional cell membrane

Figure 4. Temperature on synthetic cell membrane
a,b,c – Graphene – solid
d, e, f - Graphene - surface

Conclusions: Beyond a biomimetic synthetic interface for personalized bio-info-applications this model brings a real size-shape relationship between the organic and inorganic nanostructures at this scale, with the size related Physics (Quantum and Bio-Quantum) proper consideration.

References:

1. E. Lacatus, Self-Assembled Biofunctionalized Graphene Oxide Models for Nanomedicine, Materials Today, DOI: 10.1016/j.matpr.2017.09.066, (2017)
2. E. Lacatus, Charge carrier transfer in functionalized biomimetic sensing nanostructures, DOI:10.1016/j.bbabo.2016.04.265, BBA - Bioenergetics Volume1857, (2016)
3. E. Lacatus, Modeling a multilayered graphene biosensing structure, Materials Today, DOI:10.1016/j.matpr.2016.06.007, (2016)