

Graphene based scaffold designed for supercapacitors

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Several studies have highlighted the possibility to modulate the capacitance of supercapacitors by changing the porosity and the surface area of the graphene-based electrodes [1,2,3,4]. Therefore, a set of realistic theoretical models for these graphene-based materials are required to investigate in more details their properties and eventually to improve them.

In this perspective, we designed and exploited an algorithm inspired to the synthesis process from graphene flakes suspended in solution to generate graphene 3D-scaffolds with given porosity and specific density, and realistic structure. The obtained 3D-graphene based (3D-GB) models, were then used to build the supercapacitor electrodes. These electrodes were composed of a 3D-GB on top of a gold slab and a mixture of ionic liquid (IL) and solvent (Figure 1, Left). Gold slab, 3D-GB and the IL/solvent mixture were treated with OPLS derived classical force field (OPLS-FF). In particular, we used GoIP-FF[5] to model the gold slab, and the OPLS-based-IL-FF recently developed by Doherty and coworkers[6] to model ILs. Graphene was treated with a polarizable OPLS derived force field developed by us. Exploiting these electrode models, a series of MD simulations were performed to describe the percolation of IL-solvent mixture into the nanoporous material (Figure 1, Right), to describe the charging and discharging processes and to characterize the nanostructure of the electric double layer (EDL) at IL/3D-GB interface.

References

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Figure

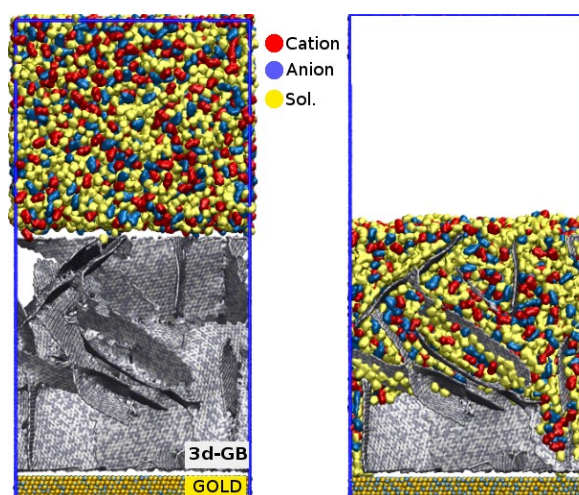


Figure 1. Left. Supercapacitor electrode model composed of a gold slab (bottom), the empty 3D-GB and the IL/solvent mixture. The cations were 1-ethyl-methylimidazolium, the anion were the bis(trifluoromethylsulfonyl) amide and the solvent molecules were the γ -butyrolactone. Right. During the MD simulation, the mixture percolates into the 3d-GB scaffold, eventually reaching the gold slab.