Graphene-based nanostructured models for hydrogen storage

Luca Bellucci
Valentina Tozzini

Nest, Istituto Nanoscienze, Piazza S. Silvestro 12, 56127 Pisa, Italy

luca.bellucci@nano.cnr.it

Graphene-based materials have generated considerable interest in the development of new nanostructured materials to be used as efficient solid-state hydrogen storage devices. Several studies have highlighted the possibility to increase the hydrogen uptake by modulating the porosity and the surface area of these graphene-based materials [1,2]. Recently, Baburin et al [3] provided experimental evidences that multilayer graphene sheets with hole defects of the order of 1-2 nm, which may be considered as a "graphene sponge", possess promising hydrogen storage capacities. Understanding the interaction mechanism between hydrogen and the irregular network of graphene sponges are therefore of paramount importance to rationalize the gas sorption process on these new systems. Nevertheless, making structures with precisely hole defects, pore size and density represents one of the major challenge in the field of nanotechnology. A set of theoretical models for the graphene sponges is thus required to investigate in more details their properties and eventually to drive experimentalists in making them.
Here we propose and implement an algorithm to generate graphene scaffold with given porosity and specific density, and realistic structure (Figure 1). The algorithm is based on a stepwise generation of graphene flakes of size, shape and orientation randomly distributed, until the wanted structural features are reached. The structure is subsequently refined by means of molecular dynamics simulations using empirical force fields. Optionally, it can be decorated with adatoms (H, O or others) to mimic the real structures generated from GO flakes or other precursors. Finally, the structure is characterized versus its gas adsorption capability by means of gran canonical monte carlo and/or diffusion molecular dynamics simulations.

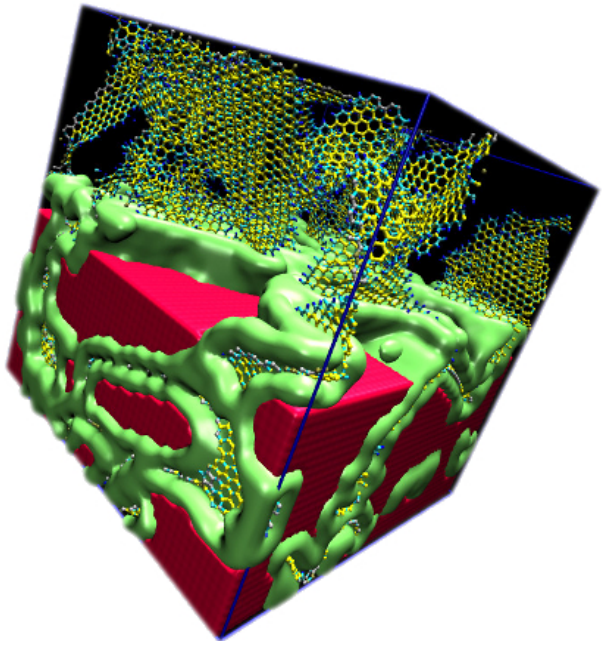

Figure1. Graphene scaffold (yellow). In green the isosurface within 3.5 Ång. from the graphene. In red large pores.

References

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