Graphene-based nanostructured models for energy storage

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Graphene-based nano-materials have generated considerable interest in the development of new nanostructured scaffolds to be used as efficient solid-state energy storage devices. For example, 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]. Understanding the interaction mechanism between chemical species (molecules, metal clusters, ions etc.) and the irregular network of the graphene based nano-structured materials are therefore of paramount importance to rationalize the properties on these new class of systems.
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. 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 hydrogen adsorption capability by means of gran canonical Monte Carlo and diffusion molecular dynamics simulations.

References

[1] S. Gadipelli, Z. X. Guo, Progress in Materials Science, 69, (2015).
[2] A. Klechikov, G. Mercier, T. Sharifi, I.A. Baburin, G. Seifertb, A.V. Talyzin, Chem. Commun., 51, (2015).

Figures

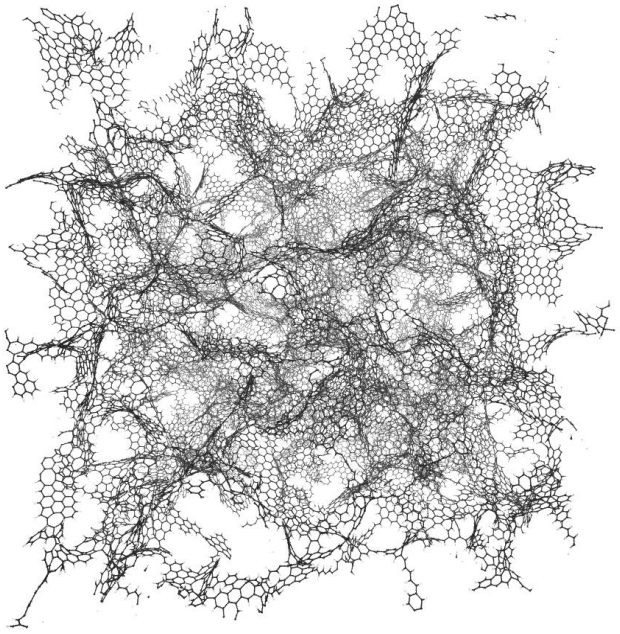

Figure 1. Example of graphene based nanostructured 3D-material.