Workshops

Chemical Energy at the Nanoscale: Simulation Meets Experiment

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Molecules and metallic nanodroplets meet carbon nanostructures

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Abstract

Carbon, with its incredibly rich variety of polymorphs, is one of the most common ingredients in novel nanostructured materials. Some of its novel polymorphs are paradigmatic of the nanoscience “revolution” (think of fullerenes, nanotubes, and graphene) with applications ranging from electronics to advanced materials passing through energy and catalysis. In many applications, it is its adequacy as a basic ingredient for the preparation porous materials what is of interest. Indeed, carbon based porous materials have a long tradition in the industry. However, the challenges of the society of the twenty first century are demanding a level of sophistication well above the traditional “activated” carbons so that novel carbon-based nanostructured materials (CNMs) are being actively studied as the next-generation of sorbents. In particular, being carbon a light element, CNMs are of interest for efficient H2 storage [1]. Nonetheless, while early experimental reports of their performance were encouraging, these have not stood the test of time. Spurred by such early results as well as by the high socio-economical impact of the field, much of the work performed in the search for carbon-based gas storage system has been based on a trial-and-error approach with rather limited results. On the other hand, the involved physico-chemical microscopic mechanisms at work are out of the realm of theoretical pillars such as the thermodynamic limit or complete long range order paramount in the “solid state” revolution of the previous century while from the numerical side, “ab inito” approaches able of dealing with the dispersive nature of the relevant interactions have been developed only recently [2]. As a consequence, a proper microscopic understanding of the associated phenomenology is still laking while whether CNMs can outperform current H2 storage technologies is still an open question.
In this talk we will present a series of studies carried out by our group (and collaborators), stimulated by the practical H2 storage problem but with an emphasis in shedding light on the microscopic mechanisms involved in the rich phenomenology associated with the CNMs as sorbents (molecular adsorption, trapping, confinement, etc). Making recourse to gas adsorption measurements, neutron scattering, and numerical modelling as the most characteristic analytic tools, we will present results regarding molecular crystallisation under nanoscale geometrical restrictions, hydrogen trapping at a molecular scale, adsorption induced 2D ordering transitions in layered CNMs and helium assisted soft landing of metallic particles onto carbon surfaces.

References

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