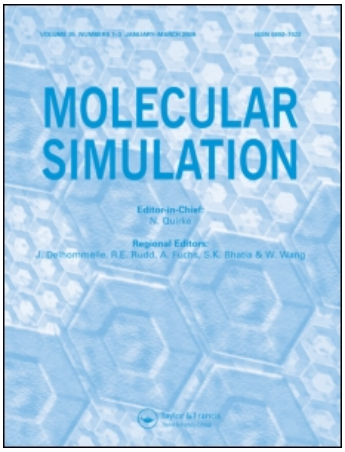

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Guest Editorial: Atomistic simulation and theory of nanoporous carbons and nanostructures

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The objective of this Special Issue is to present various modern aspects of computer simulation applied to the study of porous and nanotextured carbon materials including zeolites, nanotubes, soot particles but also more conventional disordered (activated or not) carbons. Carbon materials are at the heart of many high-tech industrial processes in electronics, aerospace technology, energy storage and filtration but are also aerosol air pollutants when emitted by cars or airplanes. It is therefore essential to acquire knowledge of the texture of these various carbon forms and related properties at the nanometric scale or even below. Carbons materials are known as very efficient adsorbents due to their high specific surface area and porosity. However the concept of pore in the real carbon materials is far from being obvious. Even in the case of carbon nanotubes that have individually a well-defined cylindrical geometry, the way by which the porosity distributes among a bundle of tubes is not yet clear. This is critical in electronic or field emission applications where dense carpets of well-aligned tubes are required. The situation gets more difficult when considering common porous carbons obtained from the thermal decomposition of organic precursors; saccharose cokes for instance. These materials all have a degree of disorder at various length scales and exhibit local nanostructures.

For characterization purposes, experimentalists use a combination of techniques that often includes low-temperature gas adsorption and transmission electron microscopy (TEM). Information from adsorption-based methods is gained assuming that the pore network can be reduced to a distribution of pores (PSD) of a given characteristic size and geometry (slit, cylinder). By contrast, TEM is a direct measure of some aspects of the material texture but 3D information such as the pore morphology (shape) and topology (the way pores distribute in space) is hard to obtain since TEM images are projections of 3D structures under an electron beam. Since the early 1970s, carboneous materials TEM data have been analysed in terms of basic structural units (graphene plane segments) of various sizes. These structural features seem common to a lot of carbon phases.

This is the reason why theoreticians have been so keen in modelling porous carbons as an assembly of slit pores of various sizes with graphitic walls of various thicknesses. Starting in the 1980s, this model was a great help in elucidating fundamental properties of confined fluids and related phenomena as a function of the pore size: micropore volume filling mechanism to capillary condensation in nanopores. These are still the subject of intense research. An objective of this Special Issue was to bring together experts in different approaches, with a view to understanding the relation between the different methods in studying and predicting adsorption properties. Several questions can be addressed. What are the strengths and weaknesses of the various available approaches and models? What are the applications for which a given approach is most suited? The reader will find in the present Special Issue several simulation and theoretical fundamental studies describing the adsorption properties of polar, non polar fluids and mixtures in slit pores or graphite surfaces (Do *et al.*, Quirke *et al.*, de Weireld *et al.*).

A few years ago, the first simulation studies of carbon porous networks not based on the slit pore model but aiming at giving some account of the real pore morphology and topology were published showing that atomistic level simulation methods can be very helpful in investigating the texture of disordered materials. However, in many cases, these also are beset with difficulties: the improvement of such atomistic approaches over the slit pore model in predicting adsorption and separation properties is not yet clear.

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The time has come to tackle this issue. The reader will find in the present Special Issue several papers on atomistic realistic models of porous carbon (Do *et al.*, Bhatia *et al.*, Biggs *et al.*) along with some simulation studies of adsorption and freezing of fluids in various realistic models of porous carbons ranging from activated saccharose cokes (Coasne *et al.*) to soot particles (Picaud *et al.*).

The last paper of this Special Issue tackles the question of the validity of one of most commonly used adsorption-based characterization method for pore PSD determination (namely the Density Functional Theory) that is available on most adsorption commercial machines (Roussel *et al.*) and routinely used in industry and research laboratories.

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