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Molecular Simulation

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Guest Editorial

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GUEST EDITORIAL

CECAM (Centre Européen de Calcul Atomique et Moléculaire) is a consortium of several European national research institutions aimed at promoting international cooperation in the field of computational physics and chemistry. A CECAM workshop was held on 11–15th September 1994 in Lyon (France), the theme of which was “Adsorption, Phase transitions and Transport in Porous Materials”. All participants in the workshop were invited to write up their presentations for publication in the present Special Issue of *Molecular Simulation*. The papers that follow provide an overview of the problems that were addressed in this meeting.

It is well known that the properties of a condensed phase can be greatly modified by its confinement. Attempts to unravel the role of geometry in changing the behavior of a molecular phase have proven to be difficult and often controversial. Confined fluids such as molecular phases adsorbed in zeolite micropores, amorphous porous materials or very thin films between two sliding surfaces have properties quite unlike their bulk.

The meeting has focused on two main challenges : 1) How to describe in a meaningful way the microstructure of the material (especially in the case of amorphous materials) and 2) how to model the external fields due to the confined geometries and understand the effect of these fields on the thermodynamics, phase transitions, structure and transport of adsorbed fluids.

Leading workers in particular topics areas were asked to review the field highlighting areas of uncertainty or controversy. This was followed by short contributions and discussion. Although many of the participants were simulators, several prominent experimentalists and theorists were invited. Further progress in this field will certainly be achieved by gathering together the questions and tools of these different researchers.

Special thanks are due to Stefano Baroni, Director of CECAM for his warm welcome and for providing us with all the facilities at Ecole Normale Supérieure in Lyon. We also wish to thank Giovanni Ciccotti, former Director of CECAM, for his help and interest in this workshop proposal.

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