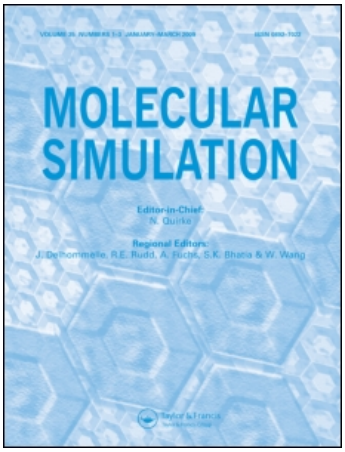

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Guest Editorial

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To cite this Article Fuchs, Alain(2004) 'Guest Editorial', Molecular Simulation, 30: 9, 559
To link to this Article: DOI: 10.1080/08927020410001717209
URL: http://dx.doi.org/10.1080/08927020410001717209

Molecular Simulation, VOL. 30 (9), 10 August 2004, p. 559

Guest Editorial

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A European Center for Atomic and Molecular Computation (CECAM, http://www.cecam.fr) workshop was held on October 2–4, 2004 in Lyon (France), the topic of which was "Molecular Simulation of Zeolites: Toward *In Silico* Design?". The co-organizers were B. Smit and A. Fuchs. The papers that follow provide an overview of the issues that were addressed in this meeting.

The topic of "Nucleation, growth and structure prediction" in zeolites has been the subject of a growing interest in the past few years. The papers of D. Vlachos and C. Mellot-Draznieck, report new and important methods such as multiscale simulations and computer designed open framework materials.

The prediction of adsorption dynamics and thermodynamics of confined phases in zeolites has been a long standing issue. The papers of J.M. Simon, F. Leroy, C. Bichara and P. Pascual provide new insights into this problem.

The effect of water on the structural properties of zeolites, with a special emphasis on the non-framework cations location is addressed by the paper of G. Maurin. Finally, water adsorption related to catalyst's acidity is the subject of the paper by F. Cora.

The progress that has been made in this field in the past decade is impressive. It was thus the right time to begin systematizing our present knowledge and analyse the areas of uncertainty and controversy.

Special thanks are due to M. Mareschal, Director of CECAM and E. Crespeau, secretary of CECAM, for their warm welcome and for providing us with the Ecole Normale Superieure facilities.

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ISSN 0892-7022 print/ISSN 1029-0435 online © 2004 Taylor & Francis Ltd
DOI: 10.1080/08927020410001717209