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Preface

This special issue on "Advanced Simulation of Materials and Catalysts" is a result of the "Molecular Modelling and Computational Methods in Catalysis" session organised by Malgorzata Witko and Roberto Millini at the EUROPACAT-IV Congress in Rimini, Italy on 6th September 1999, and a "Material Simulation for the 21st Century" symposium organised by William A. Goddard III and Peter-Paul Knops-Gerrits in the Arenberg castle of the Catholic University of Leuven, Belgium on 3rd August 1999. The special issue contains papers of the speakers at these symposia investigating structural and mechanistic properties at the atomic and molecular level of new materials and catalysts. Theoretical tools prove valuable to study new routes to the molecular engineering of materials and catalysts. Process simulation and design benefits from a new strategy for PSD software design in which the results of atomistic simulations are used to determine the activity coefficients, phase diagrams and other properties required for chemical engineering simulation and design.

Force fields involve averaging over the electronic wavefunctions to obtain parameters involving only the atoms, enabling the use of molecular dynamics (Newton's equations) rather than the Schrodinger equation. Our focus is on using data from quantum mechanics. High capacity molecular dynamics, having replaced the QM with a force field, the dynamical motions are described using Newton's equations, and high capacity simulation of 100,000–1,000,000 atoms for finite molecules or 100,000–1,000,000 atoms per unit cell for crystals and amorphous systems are new goals. Developing and validating tools for new approaches to biocatalysis and biotechnology using the techniques of macromolecular simulation to design completely new (bio)catalysts, redesign old systems so as to be stable at higher temperature or in new solvents or on new supports, test the design concepts through computer simulations, and provide data to facilitate validation of the design through experimental tests. New oxide or phosphate based materials such as aluminosilicate (zeolites) and aluminophosphate sieves and carbon materials such as carbon fullerenes and tori attract attention in this issue. In catalysis, adsorption of mono- and diatomic and larger substrate molecules preceeds and follows their transformation at the active site. Dynamics within the materials, such as diffusion in the pores of zeolites, and reactivity in acid catalysis, hydrolysis, oxidation and reduction reactions can be probed by theory using ab initio and force filed theoretical tools. The molecular, atomic and orbital description of catalytic activation and reaction mechanisms of homogeneous metal complexes as well as heterogeneous metal containing catalysts are active fields of research. Approximation of the transition structures embedded in the catalyst continuum by QM/MM methods, the properties of materials such as electronegativities, hardnesses, charges and dipole moments of the atoms in molecular sieves, the electronic levels of materials by transformation of the Brillouin zones for given topologies, the static simulation using molecular docking and the molecular dynamics calculations at various temperatures to model adsorption and diffusion, respectively, are a list of topics addressed in this volume. We hope, the reader will enjoy these advances of theory to catalysis.

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