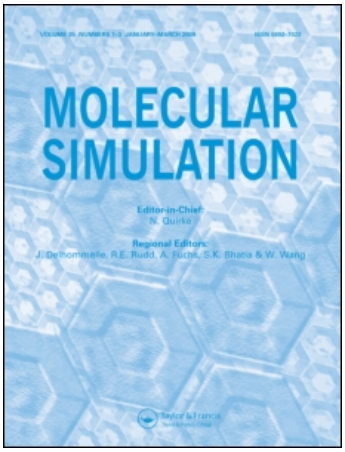

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Guest Editorial

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Guest Editorial

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Chemical reactions are often carried out under conditions that make detailed experimental investigations difficult or impossible. Examples include reactions in confined systems, such as porous media, nano-scale channels, or reverse micelles; reactions in supercritical fluids; and diffusion limited reactions, all topics of current interest. Electronic- and atomistic- level simulation methods can be very helpful in investigating such problems. However, in many cases these also are beset with difficulties. *Ab initio* methods are needed to determine the potential and free energy surfaces, and the reaction mechanism, but cannot handle more than a small number of atoms and very short times, and for some reactions the accuracy needed may be at or beyond the limit of what is attainable. The *ab initio* calculations can be used in conjunction with atomistic simulation methods, but since the reaction events are rare, specialized dynamical methods are required. Problems can also arise due to mixed ensembles. Methods for simulating chemical reactions include full scale *ab initio* methods — density functional theory, Møller-Plesset Perturbation, Coupled Cluster, Multireference Self-consistent Field, and other methods, as well as Car-Parinello Molecular Dynamics — and atomistic methods, such as Transition State Theory, "Blue Moon" Molecular Dynamics and other rare event methods, Transition Path Sampling, Reactive Ensemble Monte Carlo (for equilibrium composition), and Stochastic MC. Many situations of practical interest require a multi-scale approach and simulations involving much larger numbers of atoms or longer time scales than are accessible by rigorous *ab initio* methods.

Although there has been a great deal of published work on chemical reactivity using a wide variety of methods, there has been little interaction between proponents of the different methods, nor comparisons or reviews of the relative strengths and weaknesses of these methods. This Special Issue was inspired by a CECAM Workshop on Multi-Scale Modeling of Chemical Reactions, held in Lyon in September 2003, to address these issues. An objective of the workshop was to bring together experts in these different approaches, with a view to understanding the relation between these methods and their role in studying different types of reactive systems. Several questions were addressed at this Workshop. What are the strengths and weaknesses of the various available approaches for such cases? What are the applications for which a given approach is most suited? How might we best construct multi-scale approaches to such situations?

This Special Issue contains papers that cover a range of *ab initio* and atomistic methods for studying reactions, and a wide range of applications. The first paper introduces the subject by reviewing the various *ab initio*, semiempirical and classical atomistic approaches, and outlines their strengths, weaknesses and areas of application.

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