Special Issue

Molecular Dynamics for Chemical Reactions

Message from the Guest Editor

The simulation of chemical reactions is the holy grail of quantum chemistry. Car–Parrinello molecular dynamics paved the way to the description of complex reactive systems, also including reactive solvents. The basis is the on-the-fly approach, treating all nuclear degrees of freedom of a molecular system at once. However, almost 40 years after the development of the Car–Parrinello method, it is still difficult to describe reaction events from first principles unless the systems are small and the reactions are ultrafast. Bridging the time scales became possible with methods for the acceleration of chemical reactions such as metadynamics and chemical flooding. Attempts have been made to reduce the computational costs by using semiempirical methods or reactive force fields. Furthermore, big biochemical systems have been treated using the QM/MM approach. We welcome submissions from all these fields; not only applications, but also reports on method developments or technical developments.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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