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Molecular Reactivity: Theoretical Study and Interpretation of Experimental Results (Volume II)

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Deadline for manuscript submissions:
30 November 2024

Message from the Guest Editors

Dear Colleagues,

This Special Issue aims to collect papers investigating recent theoretical and experimental efforts exploiting new insights, methods, and techniques applied to the study of the microscopic dynamics of elementary chemical reactions. In particular, an overview of the most powerful calculation methods currently available will be published for the identification and characterization of the nature and strength of intermolecular interactions able to describe chemical reactivity. Topics include reactions between neutral species of interest in combustion, including ion–molecule reactions and those involving excited and radical species, from processes relevant for surface physics to the fundamentals of gas-phase stereodynamics, up to the physical chemistry of plasmas, planetary ionospheres, and astrochemistry, as well as complex systems of biochemical interest.

Keywords: potential energy surface; molecular reaction dynamics; theoretical chemistry ab initio calculations; combustion; astrochemistry; astrobiology; atmospheric chemistry; catalysis; calculation of kinetic parameters; modeling dust and icy grain structures and properties

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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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