Special Issue

Advances in the Theoretical and Computational Chemistry

Message from the Guest Editors

Reactivity, along with its structure, is at the core of chemistry, and is still a challenge because as the molecular or supra-molecular systems become more realistic and include explicitly more reactive environmental effects, electron transfer or photo-excitation processes, and cooperative interactions, theoretical chemistry needs to develop new approaches and algorithms to model, explain, or predict the reactivity within these systems. This Special Issue aims to provide a forum for the dissemination of the latest information on new computational and theoretical methods to describe and understand chemical reactivity.

Guest Editors

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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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