Special Issue

Combined Quantum Mechanical and Molecular Mechanical Methods and Simulations II

Message from the Guest Editors

This Special Issue of Molecules, “Combined Quantum Mechanical and Molecular Mechanical Methods and Simulations II” presents both recent developments and applications in the exciting field of multiscale computer simulations and modelling of biological systems. The purpose of this Special Issue is to showcase state-of-the-art examples of molecular dynamics simulations from quantum to classical approaches (both at atomistic and coarse-grained level), spanning a wide range of length and time scales. Both hybrid methods using two levels of resolution (such as QM/MM) and bottom-up/top-down approaches (integrating data from simulations at different levels) will be considered. Discussion about the existing challenges and problems in the is also covered, with special focus on sampling and force field limitations to describe complexity in biological systems, as well as the difficulties for the development and deployment of computational tools to assist the design and interpretation of experimental studies.

Guest Editors

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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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