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Combined Quantum Mechanical and Molecular Mechanical Methods and Simulations

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Message from the Guest Editors

Combined quantum-mechanics/molecular-mechanics (QM/MM) is an important component of many methods for in multi-scale modelling and simulations. The algorithms involve partitioning an entire system into a small subsystem of primary interest, which is modeled by an accurate QM level of theory, and the surroundings that interact with it, which are treated by MM force fields for computational efficiency. The surroundings may include the less active part of a large molecule, the solvent, all or part of a protein, or more than one of these—or other possibilities. The integration of QM and MM methods makes it affordable to realistically describe reactions in complex environments. QM/MM has found applications in many research fields such as enzymatic reactions and other catalytic reactions, ion solvation and transport, photochemistry, nanostructured materials, etc.

This Special Issue of *Molecules*, "Combined Quantum Mechanical and Molecular Mechanical Methods and Simulations," presents both recent developments and applications in this exciting field.

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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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