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The Application of Quantum Mechanics in Reactivity of Molecules II

Guest Editor:

Dr. Sérgio F. Sousa
UCIBIO/REQUIMTE, BioSIM - Departamento de BioMedicina, Faculdade de Medicina da Universidade do Porto, 4200-319 Porto, Portugal

Deadline for manuscript submissions:
closed (20 June 2022)

Message from the Guest Editor

Dear Colleagues,

Over the last few decades, the increase in the computational resources, coupled to the popularity of competitive quantum mechanics alternatives (particularly DFT), has promoted a widespread penetration of quantum mechanics calculations in a variety of fields targeting the reactivity of molecules.

The present Special Issue aims to explore this diversity of application of QUANTUM MECHANICS, including ab initio, semi-empirical, DFT, and post-Hartree–Fock methods, in the study of the electronic structure of molecules and their reactivity.

This Special Issue invites researchers to submit original research papers and review articles related to any chemical problem to which quantum mechanics has been applied. The topics of interest include but are not limited to:

- Development and application of QM methods;
- QM studies on catalysis;
- QM studies on magnetic systems;
- QM studies on excited states;
- QM studies on transition metal chemistry;
- QM studies on organic chemistry;
- QM and QM/MM studies applied biological systems;
- Quantum dynamics;
- New or improved quantum mechanical methods;
- Software programs featuring QM codes.

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Editor-in-Chief

Prof. Dr. Giulio Nicola Cerullo
Dipartimento di Fisica, Politecnico di Milano, Piazza L. da Vinci 32, 20133 Milano, Italy

Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal *Applied Sciences* has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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Applied Sciences Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

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