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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, Porto, Portugal

sergiofsousa@med.up.pt

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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.