Special Issue

The Application of Quantum Mechanics in Reactivity of Molecules

Message from the Guest Editor

The present Special Issue aims to explore this diversity of application of quantum mechanics—including ab inition, semi-empirical, DFT, and pos-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

Dr. Sérgio Filipe Sousa

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closed (30 June 2020)

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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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