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Editorial

Special Issue on "The Application of Quantum Mechanics in Reactivity of Molecules"

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Over the last few decades, the increase in computational resources, coupled with the popularity of competitive quantum mechanics alternatives (particularly DFT (Density Functional Theory methods)), has promoted the widespread penetration of quantum mechanics applications into a variety of fields targeting the reactivity of molecules. This Special Issue attempts to illustrate the conceptual diversity of the applications of quantum mechanics in the study of the electronic structure of molecules and their reactivity. It is composed of eight selected articles, of which two are review articles.

The article by Nandi et al. [1] describes the implementation of a computer program for the chemical kinetics of multi-step reactions and its integration with the graphical interface of the Virtual Multifrequency Spectrometer tool. This program is based on the ab initio modeling of the molecular species involved and adopts the transition-state theory for each elementary step of the reaction. A master-equation approach accounting for the complete reaction scheme is adopted. Some features of the software are illustrated through specific examples.

Brovarets et al. [2] addressed the conformational diversity of the quercetin molecule, an effective pharmaceutical compound of plant origin. In particular, the authors employed DFT(B3LYP) and MP2 to investigate the conformational mobility of quercetin, focusing on the rotation of the hydroxyl groups in the 3′ and 4′ positions. New pathways associated with the transformations of the conformers of the quercetin molecule into each other and associated with the torsional mobility of the O3′H and O4′H hydroxyl groups are described, highlighting the dynamical nature of this molecule.

Moubarak and co-workers [3] investigated the geometry and vibrational behavior of selenocysteine [NiFeSe] hydrogenase isolated from *Desulfovibrio vulgaris Hildenborough* using a hybrid quantum mechanical (QM)/molecular mechanical (MM) approach. The authors employed DFT (BP86 functional) to describe the QM region and CHARMM36 for the treatment of the remainder of the enzyme (MM region). The results provide an explanation for the experimental vibrational spectra, suggesting a mixture of conformers and Fe^{2+} and Fe^{3+} oxidation states.

The study by Muraro et al. [4] examined, through quantum mechanics, the antioxidant and scavenging activity of fluoxetine, a well-known and widely prescribed antidepressant drug. In particular, the authors employed the semi-empirical quantum mechanical method GFN2-xTB for conformational analysis, while the characterization of the intermediates was performed using DFT (M06-2X density functional) and SMD to account for the solvation effects. The results suggest that the antioxidant capacity of fluoxetine is due to its efficiency in increasing the concentration of free serotonin, and not due its direct ROS scavenging activity.

The article by Nalewajski [5] discussed phase equalization, charge transfer, information flows and electron communications in donor–acceptor systems, exploring the mutual relationship between the phase component of the electronic wavefunction and its current descriptor.

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Khaoaulaf et al. [6] studied the electronic structure and mechanical and optical properties of five pyrophosphate crystals with very complex structures. For that, the authors employed first-principles density functional theory calculations with different density functionals and used the results to understand and rationalize the structure and properties of those complexes, providing important clues for the understanding of pyrophosphates.

Chilukuri et al. [7] present a detailed review on the use of periodic density functional theory (PDFT) calculations in the study of the structure, electronic properties and reactivity of porphyrins on ordered two-dimensional surfaces and in the formation of nanostructures. In particular, the authors focused on examples of the application of PDFT calculations for bridging the gaps in the experimental studies on porphyrin nanostructures and self-assembly on 2D surfaces, also illustrating the diversity in terms of the density functionals used.

Finally, Nalewajski [8] reviewed different applications of quantum mechanics and information theory to problems of chemical reactivity. Particular emphasis was placed on the equivalence of variational principles for the constrained minima of the system's electronic energy and its kinetic energy component.

Together, these eight contributions constitute a rather diverse collection on the applications of quantum mechanics in the reactivity of molecules, presenting very distinct examples of applications and of perspectives, highlighting the growth and multiplicity of the field.

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