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Editorial

Symmetry in Quantum and Computational Chemistry: Volume 2

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The problem of symmetry in quantum and computational chemistry is a paradigm of development in this field of knowledge. Modern ab initio and semi-empirical methods, as well as density functional theory, widely use the group theory formalism for investigations of the nature and various properties of different periodic chemical systems (crystalline solids, polymers, surfaces and films, nanotubes) and molecules. Researchers in various fields of theoretical chemistry and related disciplines (physics, crystallography, mathematics, computer software development) are welcome to submit their works on this topic in our Special Issue "Symmetry in Quantum and Computational Chemistry, volume 2".

The aim of this Special Issue is to highlight and overview modern trends and attract the attention of the scientific community to the problem of symmetry in quantum and computational chemistry. All types of papers (reviews, mini-reviews, full papers, short communications, technical notes, and highlights) are welcome for consideration.

Our first volume of Special Issue "Symmetry in Quantum and Computational Chemistry" ran successfully and, in this Editorial, I would like to briefly highlight the papers published there.

In [1], the development of an algorithm for water molecules' symmetrical packing in the closed space of a rectangular parallelepiped was highlighted (the question regarding the closest symmetrical packing of chemical substance species (molecules, ions, polymer chains, nanoparticles, etc.) is a subproblem when predicting the structure of matter, particularly the structure of a crystal, regarding information that makes it possible to predict almost all of its properties, and the design of mathematical models for the closest symmetrical packing is an important and a challenging task in the practical application of optimization theory in theoretical chemistry). In [2], a characterization of the $E\otimes e$ Jahn–Teller (a spontaneous symmetry-breaking phenomenon, also known as a case of conical intersection) potential energy surfaces by differential geometry tools was presented. In [3], a synthesis of 2-pyridyltellurenyl bromide via Br_2 oxidative cleavage of the Te–Te bond of dipyridylditelluride was reported, and a single-crystal X-ray diffraction analysis of 2-pyridyltellurenyl bromide demonstrated that the Te atom of 2-pyridyltellurenyl bromide was involved in four different noncovalent contacts (Te$\cdots$Te, Te$\cdots$Br, and Te$\cdots$N), forming a 3D supramolecular symmetrical framework. In [4], an encapsulation of rhodamine 6G dye molecules affecting the symmetry of supramolecular crystals of melamine–barbiturate was discussed. In [5], a theoretical study of bonding and atomic charges, as well as a reactivity analysis for *closo*-borate symmetrical anions $[B_nH_n]^{2-}$ (n = 5–12), was presented. Finally, in [6], symmetrical noncovalent Br$\cdots$Br interactions were observed in the crystal structure of exotic primary peroxide.

We believe this renewed Special Issue will attract even more high-quality papers!

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