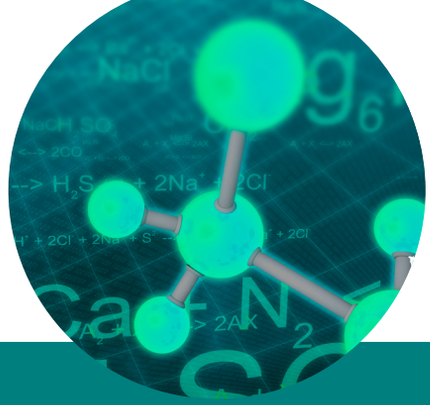
molecules

Special Issue



Quantum Information in Molecular Structures and Nanosystems

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mdpi.com/si/molecules/structures-nanosystems

Dear Colleagues,

Due to the current tremendous demand for new functional and non-toxic chemical compounds and materials for everyday life and technology, pharmacy and environmental prevention, energy harvesting, etc., the cross-fertilization of natural disciplines such as mathematics, physics, chemistry, and biology should be applied using inter- and trans-disciplinary approaches with an aim of optimizing the design–synthesis–application process : From polycyclic aromatic hydrocarbons to fullerenes, from sol-gel techniques to graphenic sheets, from topological defects to phase transitions, from chemical reactivity to biological activity and to eco-toxicity of a given target molecule or of a class of similar compounds. Manifested properties of concerned molecules and nanostructures are basically controlled, predicted and functionalized by employing the basic quantum structure principles and of allied properties regarding evolution, transfer and interaction of electrons and atoms in molecules, biomolecules, and of their nano-aggregates. Quantum-nano-information becomes therefore the true playground by which the qualitative-quantitative conceptual-functional "jump" rather than "just progress" may be achieved aiming for the betterment of life in the long run, and, in the interim, analyzing functional molecular integrated-systems for special applications (e.g. deposition, transferring, amplifying, converting and controlling the macro-material information through their nano-molecular structural properties). The objective of this Special Issue is in gathering the basic, as well as frontier approaches, of quantum information and molecular topology for single, ribbon and extended nano-molecular systems, in reciprocal equilibrium and dynamics, already synthesized or virtually designed.

Dr. Dr. Habil. Mihai V. Putz

Guest Editor

Special Issue Topics:

- quantum information theory, shapes of atoms-in-molecules
- new chemical bonding paradigms
- nanostructures and topological defects
- reactivity and topological indices
- crystallography; computational chemistry
- molecular and nanostructure design
- nanostructure synthesis and quantum characterization
- aromaticity

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