symmetry

MDPI

Editorial

Symmetry in Quantum and Computational Chemistry

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Symmetry is a paradigm of quantum and computational chemistry (Figure 1). Modern ab initio (Hartree–Fock methods (HF), Møller–Plesset perturbation theory (MP*n*), configuration interaction (CI), coupled cluster (CC), quadratic configuration interaction (QCI), quantum chemistry composite methods (G2, G3, G4, T1, the Feller–Peterson–Dixon approach, the correlation consistent composite approach, complete basis set methods, Weizmann-*n* theories), multi-configurational self-consistent fields (MCSCF, including complete active space self-consistent field (CASSCF) and restricted active space self-consistent field (RASSCF)), multi-reference configuration interaction (MRCI), n-electron valence state perturbation theory (NEVPT), complete active space perturbation theory (CASPT*n*), state universal multi-reference coupled-cluster theory (SUMR-CC)) [1] and semi-empirical methods (Pariser–Parr–Pople method (PPP), complete neglect of differential overlap (CNDO), intermediate neglect of differential overlap (INDO), neglect of diatomic differential overlap (NDDO), modified intermediate neglect of differential overlap (MINDO), modified neglect of diatomic overlap (MNDO), Austin model 1 (AM1) and its reparameterized modification, Recife Model 1 (RM1), parametric method 3 (PM3) and its reparameterized modifications (PM6, PM7), semi-empirical ab initio model 1 (SAM1), Zerner's intermediate neglect of differential overlap (ZINDO)) [2], as well as density functional theory (classical [3] and relativistic [4], as well as time-dependent [5] DFT) all widely use group theory formalism for the investigation of nature and various properties of different periodic chemical systems (crystalline solids, polymers, surfaces and films, as well as nanotubes) and molecules.

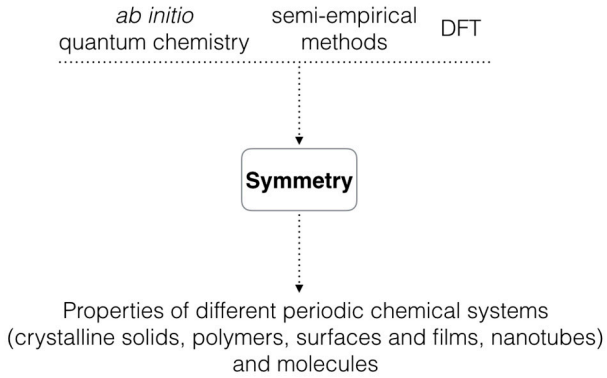

Figure 1. Symmetry is a paradigm of quantum and computational chemistry.

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, highlights, etc.) are welcome for consideration.

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