

Special Issue

Simple Substances of Non-metals: Molecular Structures Modeling with Using DFT and More Advanced Methods of Quantum Chemistry

Message from the Guest Editor

Dear colleagues, This Special Issue aims to include mainly original full articles and short messages devoted to quantum-chemical calculations of the molecular structures of polynuclear simple substances formed by non-metals of p -elements (both neutral and polynuclear monoelement cations and anions). This mainly concerns polynuclear simple substances formed by carbon atoms, nitrogen, phosphorus, oxygen and sulfur; however, articles devoted to polynuclear simple substances and of other non-metallic elements (boron, silicon, arsenic, etc.) can also be submitted for publication in this Special Issue. We welcome articles in which, along with the required quantum-chemical calculations, experimental data will also be presented to evaluate the reliability of these calculations. Review articles may also be submitted for publication in this Special Issue (including author reviews, the emphasis of which is mainly on the work of their authors).

Guest Editor

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Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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