

Special Issue

Molecular Structure, Electronic and Vibrational Spectra Theoretical Calculations in Materials Sciences

Message from the Guest Editor

The dialectic of the development of science is expressed in the fact that today's experiment must give way to tomorrow's theory, which makes this experiment unnecessary, but which, in turn, must give way to a new, more accurate experiment the day after tomorrow, and so on.

The problem along this path is the different physical meaning of the molecular parameters obtained in experiment and in quantum chemical calculations. We are pleased to invite you to present your works in this Special Issue, which considers examples of the joint use of experimental and calculated data and the problems that arise in this connection. **Keywords**

- molecular structure
- nature of chemical bonding
- IR spectra
- EA spectra
- NMR
- XRD
- DFT
- ab initio

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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