



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

Guest Editor:

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Message from the Guest Editor

Dear Colleagues,

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





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Message from the Editor-in-Chief

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