

Special Issue

Quantum Chemistry as Applied to Molecular Systems

Message from the Guest Editor

Quantum chemical calculations are an integral part of contemporary chemistry and are used to support experimental work in virtually every part of the discipline. The accuracy of the calculations has improved steadily while the knowledge, tools, and expertise have been passed from specialist to general user. The result has been improved understanding, accelerated discovery, and facilitated optimisation of molecules, molecular materials, and interfaces. This Special Issue seeks to coordinate recent advances in quantum chemical methodology in the general field of molecular science. Emphasis is given to quantum chemical studies of molecular associates, such as dimers, in both ground and excited states and in developing new tools to aid spectroscopic investigations. Both excitonic and vibronic couplings are now addressable by theoretical methods, while the involvement of charge transfer or extended p-conjugation in large organic molecules merits special attention. The study of delocalised organic radicals, such as those derived from cyanine dyes, is necessary for an improved understanding of super-resolution microscopy. Manuscripts covering related topics are welcome.

Guest Editor

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Deadline for manuscript submissions

closed (31 March 2024)



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About the Journal

Message from the Editor-in-Chief

Symmetry is ultimately the most important concept in natural sciences. It is not surprising then that very basic and fundamental research achievements are related to symmetry. For instance, the Nobel Prize in Physics 1979 (Glashow, Salam, Weinberg) was received for a unified symmetry description of electromagnetic and weak interactions, while the Nobel Prize in Physics 2008 (Nambu, Kobayashi, Maskawa) was received for the discovery of the mechanism of spontaneous breaking of symmetry, including CP symmetry. Our journal is named *Symmetry* and it manifests its fundamental role in nature.

Editor-in-Chief

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