

Special Issue

Computational Chemistry in Nuclear Magnetic Resonance

Message from the Guest Editor

Dear Colleague, Accurate quantum chemical modeling of NMR spectra is deeply involved in the NMR structural assignment of compounds that are currently of utmost importance in both organic and inorganic chemistry. The development of new effective approaches and computational tools capable of providing very accurate NMR chemical shifts and spin-spin coupling constants is at the cutting edge of modern computational NMR spectroscopy. Since the first application of perturbation theory to NMR properties by Ramsey over 70 years ago, computational methodology has taken a great strides due to both the accelerated progress of computer techniques and the development of electronic theory. This Special Issue entitled *Computational Chemistry in Nuclear Magnetic Resonance* will provide researchers with the opportunity to publish their most recent discoveries in the field of high-quality computational methodologies relating to NMR spectral parameters. Dr. Irina L. Rusakova

Guest Editor

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About the Journal

Message from the Editor-in-Chief

Magnetochemistry constitutes a multidisciplinary field where chemists and physicists not only study magnetic properties but also design and synthesize chemical compounds with desired magnetic properties.

Magnetochemistry is inviting contributions in any field related with this area, such as theoretical models, crystal engineering, molecular magnetism, SMM, SIM, SCM, SCO, magnetic nanostructures, magnetic MOFs, magnetic recording, qubits, magneto-caloric materials, etc. Our goal is to share your contribution in a timely fashion and in a manner that will be valued by the scientific community.

Editor-in-Chief

Prof. Dr. Carlos J. Gómez García

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