

Special Issue

Computational Modelling of Magnetic Molecules and Multifunctional Magnetic Materials

Message from the Guest Editor

The field of computational modelling of magnetic materials is witnessing exciting times. Now more than ever, with the increasing efficiency and accuracy of ab initio simulations and the advent of machine learning methods, computational sciences are at the forefront of scientific innovation. Quantum chemistry has played a fundamental role in the advances in molecular magnetism and it remains a fundamental force driving the design of new magnetic materials. However, many different computational disciplines are now needed to provide a comprehensive understanding of complex and dynamic magnetic phenomena. Theory and modelling of spin relaxation, spin transport, and molecular dynamics are only a few of the many fields of growing interest for the communities working on magnetic materials and spin-based quantum technologies. This Special Issue aims to provide an overview of the many branches of the state-of-the-art advances in this rapidly evolving field and it aspires to showcase the most important advances in the computational modelling of magnetic molecules and multifunctional magnetic materials.

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

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