magnetochemistry

an Open Access Journal by MDPI

IMPACT FACTOR 2.6

CITESCORE 3.9

Computational Modelling of Magnetic Molecules and Multifunctional Magnetic Materials

Guest Editor:

Dr. Alessandro Lunghi
School of Physics, Trinity College Dublin, Dublin 2, Ireland

Deadline for manuscript submissions:
closed (20 December 2021)

Message from the Guest Editor

Dear Colleagues,

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.