

Special Issue

Theory and Simulations of Single-Molecule Magnets

Message from the Guest Editor

Molecular magnets are systems with a series of transition metal atoms surrounded by ligands. The magnetic properties of these molecules, which can be used to design magnetic storage and spintronic devices, depend on the interplay between properties such as super-exchange, spin-orbit coupling, and the crystal field. The correct prediction of these properties using ab initio methods is, however, not easy, and theoretical results often differ from experimental ones. In this issue, we cover the latest developments of simulations of single-molecular magnets using ab initio methods.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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