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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