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Theory and Simulations of Single-Molecule Magnets

Guest Editor:

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Deadline for manuscript submissions:
closed (15 June 2021)

Message from the Guest Editor

Dear Colleagues,

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.

Prof. Dr. Victor M. García-Suárez
Guest Editor

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Message from the Editor-in-Chief

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