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Electronic Structure Calculations Applied to Magnetic Phenomena

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Message from the Guest Editor

Dear Colleagues,

The use of transition metal complexes with magnetic properties in the design of nanoscale based devices remains one of the most active research fields in Inorganic Chemistry, both from the experimental and theoretical points of view. As a matter of fact, the use of electronic structure based calculations to gain further insight into the origin of these properties has been crucial in the rational design of new molecules with tailored properties. Using computational tools, it is possible to underline the electronic structure origin of key parameters in magnetic systems such as anisotropy terms, exchange coupling constants or transition temperatures in Spin-Crossover systems. This type of calculations are crucial to understand both the origin and trends of such properties in these systems.

This Special Issue of *Molecules* highlights both recent developments and applications of electronic structure methods in the fields of Single Molecule Magnets (SMMs) and Single Ion Magnets (SIMs), Spin-Crossover systems and magnetically ordered systems among others.

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th 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 multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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