Theory meets Experiments: the Case Study of the Bistable Dithiazoxylyl-based Molecular Magnets

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L’ organizzatore
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Theoretical predictions of magnetic properties of bistable purely organic molecule-based magnets have experienced an incredible progress during the last years. Our attention is focused on dithiazolyl (DTA)\textsuperscript{1,2} compounds, being promising candidates for potential technological applications (e.g. storage devices, quantum computers, etc.). In this talk, the theoretical approaches aimed at identifying the magnetic topology of the molecular crystals,\textsuperscript{3} as well as the structural vs. electronic factors affecting the magnitude of the overall radical···radical $J_{ab}$ magnetic coupling, will be presented. Particular emphasis will be put on the support that computational models and techniques can provide in the quest for tailored properties in the material design. We will present magneto-structural correlation maps as a function of the substituents of the DTA-moiety to highlight which is the static ferromagnetic fingerprint region.\textsuperscript{4} Finally, if time permits, an alternative mechanism for inducing spin transitions in materials based on planar organic radicals will be shown by means of a combination of static and dynamical analysis.

**Figure 1.** Comparison between experimental (◼) and computed (◼/◼) susceptibility curves for the low temperature (LT) and high temperature (HT) phases of PDTA and TDPDTA systems. In particular, here the reported the results for the best 1D models for both the polymorphs considered in both materials.

**References**