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IL DIPARTIMENTO DI SCIENZE MOLECOLARI E NANOSISTEMI

VI INVITA AL SEMINARIO :

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

Tommaso Francese

Dept. Ciència de Materials i Química Física &
IQTCUB, Universitat de Barcelona
& Zernike Institute for Advanced Materials,
University of Groningen

May 7th, 2019
12:00 Conference Room

L' organizzatore
prof. Pietro Riello

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

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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)[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,[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[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.

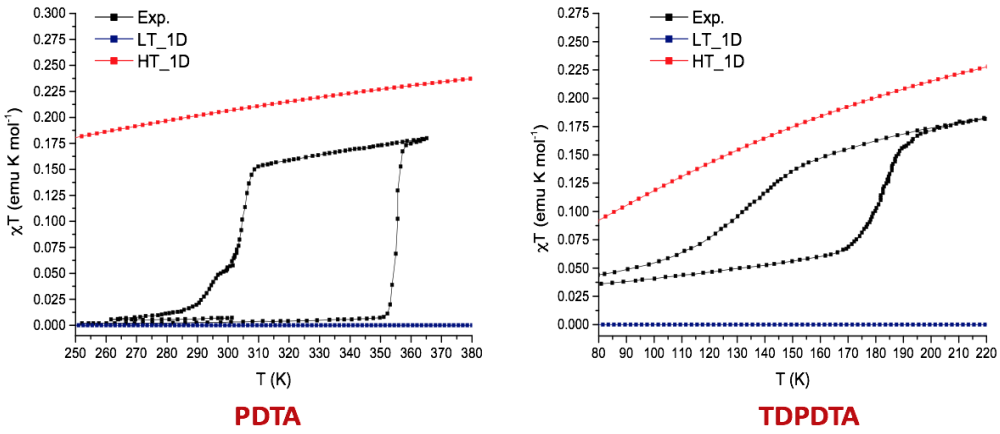


Figure 1. Comparison between experimental (■) and computed (■/■) susceptibility curves for the low temperature (LT) and high temperature (HT) phases of PDTA and TDPDTA systems. In particular, here the reported the results for the best 1D models for both the polymorphs considered in both materials.

References

[1] Brusso JL., *et al.*, Bistabilites in 1,3,2-dithiazolyl radicals, *J. Am. Chem. Soc.*. **126**, 8256-8265 (2004);

[2] Vela S., *et al.*, Bistability in Organic Magnetic Materials: A Comparative Study of the Key Differences between Hysteretic and Non-hysteretic Spin Transition in Dithiazolyl Radicals, *Chem. Eur. J.*, **23**, 3479 – 3489 (2017);

[3] Vela S., *et al.* Towards an accurate and computationally-efficient modelling of Fe(II)-based spin crossover materials, *Phys.Chem.Chem.Phys.*, **17**, 16306 (2015);

[4] Francese, Tommaso, *et al.* "The magnetic fingerprint of dithiazolyl-based molecule magnets." *Phys. Chem. Chem. Phys.* **20.31**, 20406-20416 (2018);