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Editorial

Special Issue "Spin Crossover (SCO) Research"

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This special issue, entitled "Spin Crossover (SCO) Research", illustrates the current relevance of a focused topic, which is in turn highly versatile. Indeed, the collection of papers presented constitutes a sampler that shows the topical importance of this area by attracting the interest of many top researchers and how it is approached under a multidisciplinary perspective.

The guest editors are thankful to the publisher and their professional editorial team, who have helped enormously in the task of putting together this issue. The serious, altruistic, and dedicated work of all the referees is also gratefully acknowledged. Finally, the generosity and the strong scientific input of the authors that have contributed their papers with some of their best research results deserve the strongest recognition.

The collection of manuscripts in this issue encompasses two high-quality review articles and eighteen outstanding research papers. Following the announced spirit of the original call, very diverse aspects of the phenomenon of spin transition are treated. Therefore, a good balance between theory, synthesis, and physical studies is encountered, while various manifestations of SCO materials are present as part of the theoretical treatments as well as experimentally (molecular, polymeric, nano-structured, and composite materials).

The issue includes Monte Carlo simulations of the dynamic properties of the SCO phenomenon analyzing the influence of crystal defects [1], the surface effects [2], and the interactions within the bulk of the system using an Ising model [3]. In addition, density functional theory (DFT) calculations are employed to study the cooperativity using a very well-known experimental compound [4]. A recently published molecular system is reevaluated also by means of DFT calculations to propose novel ligand effects to the low/high spin relative stability [5], while this method is also employed in combination to nuclear inelastic scattering (NIS) data to unveil the coupling between the vibrational levels near one Fe(II) center, with the neighboring centers depending on the relative spin states [6].

This special issue also witnesses the synthesis of new SCO systems and their properties. These include a family of Fe(II) complexes with a new 4-hydroxy 1bpp ligand (1bpp; 2,6-di(pyrazol-1-yl) pyridine) [7], two derivatives of the alkyl-*1H*-tetrazole series, now exhibiting a propargyl function as a way to perform post-synthetic modifications of SCO compounds [8], and a novel series of Fe(III) heteroleptic molecules exhibiting varying magnetic behaviors, explained in terms of differing types of intermolecular interactions [9]. Abrupt SCO of another series of Fe(III) molecules combining imidazole and Shiff-base related ligands is also explained as a result of hydrogen bonding interactions propagated in one direction of the crystal lattice [10]. A novel Fe(II) mononuclear species made with a pyridylmethyleneaniline ligand featuring an isopropyl group exhibits hysteresis resulting from the coupling of the SCO transition with a process of conformational isomerism of the latter substituent [11]. In addition to mononuclear systems, this issue channels the presentation of a novel trinuclear spin transition complex [12].

A series of papers underline the importance of advanced physical studies of existing compounds for the progress of the field. A remarkable case is made by the study on the effect of external pressure on a SCO complex, unveiling the coupling between the structural changes associated with the spin transition and the concomitant change to the dynamical disorder of the counter ion [13]. In relation to this, another remarkable study shows the effect and differences to the hysteresis of a known highly cooperative compound of in situ and ex situ external pressure, as well as internal pressure (the latter by introduction of different percentages of an isostructural Mn(II) complex into the lattice of the Fe(II) SCO species) [14]. The intriguing relaxation dynamics that a rare trinuclear complex with a very wide hysteresis loop exhibits of its metastable HS state, is presented and quantified [15]. The potential of chemical sensing that many SCO compounds have of small molecules, thanks to their switching properties, is featured in this special issue as well [16].

Representative of the importance and growing interest in manipulating and shaping molecular-based SCO materials at the nano-scale are two interesting papers. One explains methodologies of preparing size- and shape-controlled nanoparticles of one archetypical SCO tetrazole-based Fe(II) polymer [17], and the other one demonstrates the effect of the cooperative spin transition in nanoparticles of the same Fe(II) polymer on the fluorescence of nanocrystals of CdTe within nanocomposite materials made of both functional systems [18].

The reviews featured in this special issue are of great topical interest. The first constitutes a revision of an aspect of SCO research that is gaining increasing interest: the crystallographic symmetry breaking that occurs as a result of the spin transition in many systems [19]. As more and more detailed information becomes available thanks to increasingly powerful crystallographic characterization techniques, more details are being recognized about the close relationship between the dynamics of SCO and the crystal lattice hosting the active materials. This review is thus of paramount importance. The other review illustrates very well the current tendency of coupling the phenomenon of SCO to the switching character of other materials properties as a powerful strategy of exploiting the magnetic phenomenon for its integration into sophisticated nanoscopic multifunctional devices [20]. Thus, the review not only revises the synergy between magnetic transitions and charge transport properties, but also emphasizes how these synergies may be implemented on nanostructured materials, such as thin films, nanoparticles, and single molecules.

We hope that this special issue will not only help to enlarge the visibility of important current figures as well as emerging players in the area of SCO, but also generate the interest of an increased portion of the scientific community for this exciting field. The fact that *Magnetochemistry* is an open access journal will certainly fit these purposes. We wish this young journal every success along the journey upon which it has just embarked.

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