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Exploring Spin Crossover Compounds for Barocaloric Application

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Barocaloric refrigeration leverages the adiabatic temperature and isothermal entropy changes of materials under external hydrostatic pressure, presenting a promising energy-efficient and eco-friendly refrigeration technology. Among the materials considered for barocaloric applications, Spin Crossover (SCO) compounds have recently gained attention due to their unique properties.

SCO compounds are characterized by a transition of the central metal ion between a low spin (LS) state, favored by low temperature and high pressure, and a high spin (HS) state, favored by high temperature and low pressure. This transition is accompanied by significant changes in entropy, which are crucial for barocaloric applications. However, understanding the microscopic mechanisms underlying the HS-LS transition remains challenging.

Our research focuses on the SCO compound $[Fe(Pm\text{-}Bia)_2(NCS)_2]$, where (Pm-Bia) stands for (N-(2′-pyridylmethylene)-4-amino-biphenyl). This compound crystallizes in two polymorphs that exhibit distinct spin state transitions. We investigate these transitions using magnetization and DSC measurements, as well as powder and single-crystal X-ray diffraction, under varying temperature (80-300 K) and pressure (0-2 GPa) conditions.

The orthorhombic polymorph of $[Fe(Pm\text{-}Bia)_2(NCS)_2]$ exhibits a sharp HS-LS transition within 1 K when subjected to temperature changes. However, applying external pressure does not induce a spin transition in this polymorph; instead, it leads to the formation of a superstructure at 2.02(4) GPa. In contrast, the monoclinic polymorph shows a gradual HS-LS transition over a broad temperature range (~100 K) and undergoes a transition to the LS state upon the application of pressure up to 1.36 GPa at room temperature.

In this study, we highlight the role of intermolecular interactions in determining the nature of the spin transition. We discuss and compare our observations in the context of cooperativity and spatial requirements, providing deeper insights into the structural changes associated with the HS-LS transitions in SCO compounds.

This research contributes to the understanding of SCO compounds for barocaloric applications, emphasizing the importance of structural analysis and the role of different perturbations on spin state transitions.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Advanced Materials & Processing