

Poster Presentation

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Structural studies of a flexible 2D layer spin crossover coordination polymer

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The first coordination sphere of spin crossover material has been comprehended to play a dominant role to its magnetic property. However, the intermolecular interactions, such as $\pi\cdots\pi$ interaction and hydrogen bonding, also play a crucial factor. The contents of the solvent in a 2D layer structure, $\text{Fe}(\mu\text{-atrz})(\mu\text{-pyz})(\text{NCS})_2\cdot n\text{H}_2\text{O}$ where $n=4, 2$ and 0 , has been reported to be able to affect the spin transition behavior dramatically.[1] As loss of solvent molecules, the inter-layer distance becomes shorter and the transition temperature shifts to lower temperature and accompanies a larger hysteresis loop. To further understand the correlation between the inter-layer distance and magnetic property, the guest ab/desorption and pressure-induced synchrotron powder diffraction experiments were performed at BL01C2 in NSRRC. Based on the cyclic TGA measurements, the guest molecules, H_2O , MeOH and EtOH , all can be removed and retaken repeatedly. The pressure-induced PXRD experiment was performed using a Boehler-Almax design diamond anvil cell (DAC). The detail structural studies attempt to understand not only the spin state changes from HS (high spin state) to LS (low spin state) but also the cooperative effect through the inter-layer distance.

[1] Y. C. Chuang, C. T. Liu, C. F. Sheu, W. L. Ho, G. H. Lee, Y. Wang, *Inorg. Chem.*, 2012, 51, 4663-4671

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