Design of Thiocyanate-bridged Multifunctional Fe^{II}-Hg^{II} Frameworks

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Numerous aspects of spin-crossover (SCO) materials, such as syntheses, structures and physicochemical properties, have been vigorously researched in last decades.[1,2] In this context, the goal of my work is to design and characterize the high dimensional thiocyanate-bridged SCO compound $\{[Fe(4\text{-acpy})_2][Hg(SCN)_4]\}_n$ **(FeHg4-Acpy)** based on iron(II) ions with $[Hg(SCN)_4]^{2-}$ anions and 4-acetylpyridines(4-acpy). Crystals of **FeHg4-Acpy** forms 3D network built of two symmetry-independent tetragonally-distorted octahedral $[Fe(4\text{-acpy})_2(NCS)_4]$ units and it crystallizes in the non-centrosymmetric orthorhombic space group $Pna2_1$. The noticeable changes of structural parameters with temperature of crystal were observed, which can be accounted to changes of spin state of central Fe^{II} ions from low spin state ($S_{Fe(II)} = 0$) at low temperature to high spin state ($S_{Fe(II)} = 2$) at high temperature. The compound is found to have fully occupied quintet paramagnetic high-spin(HS) state in two Fe^{II} sites at 300 K. When cooling down, it revealed partial SCO effect with $T_{1/2}$ = 103 K owing to the formation of low-spin state for one Fe^{II} ion ($S = 0$, $t_{2g}^6 e_g^0$) and high-spin state for another Fe^{II} ion ($S = 2$, $t_{2g}^4 e_g^2$). The Light-Induced Excited Spin-State Trapping (LIESST) effect can be observed for this crystal with 473, 532, 658 and 1064 nm lights, which can be further confirmed by temperature-dependent UV-Vis, IR and THz-TDS spectroscopy.

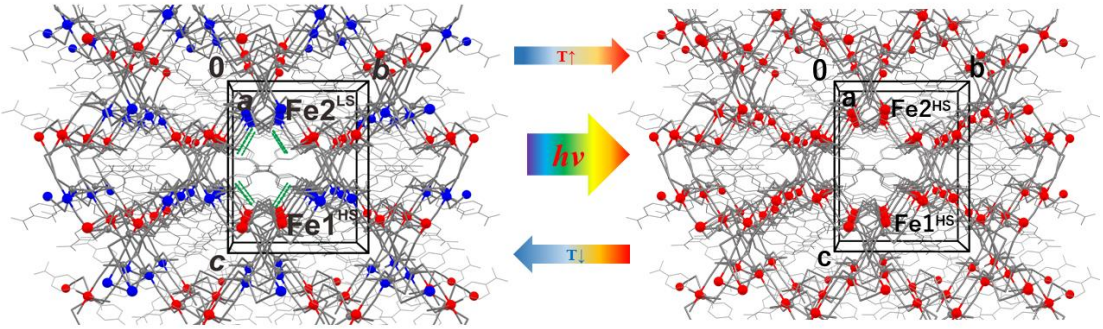

Figure 1. Structures of **FeHg4-Acpy** at 90K(*Left figure*) and 300K(*Right figure*)

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