Poster Presentation

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Characterization of Pressure-induced Phase Transition on [Co(bpy)3](NO3)2•3H2O

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The pressure-induced phase transition study of high-spin (HS) compound, [Co(bpy)3](NO3)2•3H2O (bpy = 2,2'-bipyridine), is characterized by powder x-ray diffraction (XRD), x-ray absorption spectroscopy (XAS), Raman spectroscopy, and theoretical calculations. The results indicate that the HS ground state t2g5eg2 on Co(II) is gradually transformed to low-spin (LS) state with configuration t2g6eg1 . This phase transition behavior is similar to the thermal-induced spin crossover phenomenon once it is incorporated into certain framework. In this study, we put the compound into diamond anvil cell and applied physical pressure to replace the framework effect. To analyze the x-ray absorption near edge structure (XANES) and Raman spectroscopy, the finite difference method for near-edge structure (FDMNES) and density functional theory (DFT) calculations are applied to illustrate the experimental spectroscopies, respectively. In XANES results, an intersection point around 7756.33 eV beyond 1.73 GPa is assigned as the critical point between HS and LS state. The extended x-ray absorption fine structure (EXAFS) analysis indicates that the averaged Co-N bond lengths is 2.127(7) Å at HS state and decreased to 1.950(4) Å at LS state. Based on XRD analysis, the external pressure reduces the hexagonal cell constants from a = 13.77(3) Å and c = 21.71(3) Å to a = 13.37(5) Å and c = 21.11(1) Å. According to those experimental results, the mechanism of such pressure-induce spin transition can be interpreted as the enhancement of intermolecular interaction by increasing the external pressure.

Keywords: spin crossover, x-ray absorption spectroscopy, powder x-ray diffraction