Keywords: Nickel phosphonates, Hydrothermal synthesis, Ab initio crystal structure determination, Thermal characterization, Magnetic characterization.

MS37-P7 Structure-versus-luminescence Reversibility and Solvent Adsorption Properties of a 3D Porous Supramolecular Metal–organic Frameworks Studied by Synchrotron X-ray Powder Diffraction

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A three-dimensional (3D) porous supramolecular architecture, {[Zn(bdc)(dpds)]·0.62(MeOH)·2H_2O}n (1), with a 2D layered-like metal–organic framework (MOF) has been synthesized. Adjacent layers are assembled via two types of π–π interactions, the sandwich-type $\pi_{pyridyl}$–$\pi_{benzene}$–$\pi_{pyridyl}$ and $\pi_{pyridyl}$–$\pi_{pyridyl}$ fashions to afford a 3D porous supramolecular architecture. Controlled heating of the as-synthesized crystal 1 at ~120 °C causes de-solvated species of {[Zn(bdc)(dpds)]}n (1a). The de-solvated compound shows the same structure as that of 1 with the nonexistence of solvated MeOH and water molecules. The de-solvated 1a generates the re-hydrated crystal of {[Zn(bdc)(dpds)]·1.1(H_2O)}n (1b) upon exposure to water. The water ab-/de-sorption phenomenon by cyclic TG measurement suggests the complete reversibility upon re-/de-hydration between 1a and 1b, associated with reversible temperature-dependent light emission properties. Moreover, 1a also displays interesting reversible water, methanol and ethanol vapor ad-/de-sorption behavior correlated with the polarity of the pore surface in 1a to the corresponding adsorbate molecules. The crystal structures of as-synthesis, dehydration and rehydration forms were studied by *in situ* synchrotron X-ray powder diffraction.

Keywords: Synchrotron Radiation, Powder X-ray Diffraction, MOF, Luminescence