ABSTRACT

TITLE:Investigation on the Functional Coordination Polymers: Synthesis, Structure and Potential Applications

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Chapter 1. This chapter is divided into two sections: Chapter **1A** focuses on a brief survey regarding coordination polymers and their functional behavior, while Chapter **1B** provides a summary of research works.

Chapter 2. A new coordination polymer, $[Cd(C_8N_2O_3H_7)_2(H_2O)_2]_n$, synthesized using a bio-inspired ligand *via* hydrothermal method, exhibited significant properties such as strong blue emission centered at 420 nm and selective sensing of p-xylene, and pH-dependent luminescence with DFT studies supporting the findings.

Chapter 3. In this chapter two new isostructural 2D polymers, $\{[Mn(PDA)(4\text{-bpdb})(H_2O)_2].4\text{-bpdb}\}_n$ and $\{[Fe(PDA)(4\text{-bpdb})(H_2O)_2].4\text{-bpdb}\}_n$, synthesized via layer diffusion, showed promising electrochemical properties with compound **1**(Mn) demonstrating higher specific capacitance and conductivity, while compound **2**(Fe) exhibited superior cyclic stability.

Chapter 4. This chapter presents a new cadmium(II)-based two-dimensional coordination polymer $[Cd(L)(NA)(H_2O)]$ (L = Iminol form of N-nicotinoyl glycinate, NA = Nicotinate), which formed a corrugated layer structure with a three-dimensional supramolecular *ABABAB*…type packing arrangement. The compound, characterized by single-crystal X-ray diffraction, powder X-ray diffraction, FT-IR spectroscopy, and thermogravimetric analysis, exhibited excellent stability in water and strong blue luminescence at 420 nm. It effectively detected sulfonamide antibiotics at parts-per-billion levels (226-726 ppb) via luminescence quenching and was also used in the fabrication of Schottky diode devices with a barrier height of 0.86 eV and an ideality factor of 1.24.

Chapter 5. A 3D cadmium crystalline network, $[Cd_3(L)_2(LH)_2(bpe)_2]$, was synthesized by layer diffusion method after that it undergoes selective post-synthetic metal ion exchange with copper in DMF solvent. Metal exchanged CNM exhibited enhanced thermal stability, red shifted emission

emission and enhanced N_2 uptake along with this parent compound showed excellent heterogeneous catalytic properties.

Chapter 6. A Ni(II) based 3D MOF and its bimetallic derivative [Ni(II) and Co(II)] synthesized via the hydrothermal method, exhibited exceptional electrocatalytic properties for hydrogen evolution reaction, highlighting the synergistic approach and potential of bimetallic MOFs in sustainable energy research. Additionally bimetallic synergy was supported by DFT.

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