Abstract

Based on the rapid growth in industrialization for human needs and comfort, one of the major programs in recent times is focused on multidisciplinary research efforts to deal with energy and environment issues. Chemistry plays a critical role in how our societies will contend with broader global effects related to such issues. For this reason, different kinds of new multifunctional materials are designed and evaluated for their possible applications in various related topics with special attention to cost and efficiency. In the past two decades, there is a giant leap in the sphere of strategic design of diverse functional materials namely supramolecular coordination assemblies, coordination polymers (CPs) and metal organic frameworks (MOFs), which are collectively termed as Metal Organic Coordination Networks (MOCNs), for various applications such as carbon capture, gas storage/separation, catalysis, sensing, water purification, drug delivery, guest encapsulation, magnetism, etc. The construction of such functional materials via coordinationdriven self-assembly of metal ions/clusters and multitopic organic linkers depends on coordination bonds and supramolecular interactions, such as hydrogen bonds, $\pi - \pi$ and/or C-H ... O interactions, etc. Through judicious choice of the components in making such coordination architectures, it is possible to generate materials with tunable structures varying dimensionality and topology and targeted physicochemical properties and functionality. This thesis work focused on the strategic designs to obtain a variety of MOCNs under ambient, hydro- or solvothermal conditions in good to high yields via self-assembly of both two-component (metal ions and custom-designed mixed pyridyl-carboxylate linkers) and three-component (metal ions, neutral ancillary ligands, and carboxylate linkers) systems. These have been extensively characterized by various analytical techniques including elemental analysis, FT-IR, Raman and UV-Vis spectroscopy, TGA, single crystal and powder X-ray diffraction, and ESI-MS analysis. Their applications in four different areas, namely (i) guest encapsulation (water clusters including rare cyclic dimers and cyclic pentamers, and common organic solvents in supramolecular coordination assemblies), (ii) ion exchange (waste water purification and separation of dyes by anionic MOFs), (iii) catalysis (cascade N-alkylation reaction and the Knoevenagel condensation reaction by Pd NPs@MOFs) and (iv) sensing (ketones, amines and nitroaromatic compounds by luminescent MOFs), have been explored to contribute tremendously to the targeted efforts sought in the multidisciplinary approach mentioned above. There are four chapters in this thesis.