Abstract [IndexNo: 153/22/Chem./28]

Title: Designing of Functional Co-ordination Polymers for diverse Applications

Coordination Polymers (CPs) or Metal-Organic Frameworks (MOF) have extensive role in the field of sensing, electrical conductivity, gas absorption, magnetism, water splitting, environmental management, drug delivery and other biological applications. Using a combination of bridging ligands and various metal nodes, coordination polymers are created. Transition metal CPs with aromatic or aliphatic carboxylate (linker) and/or N-heterocyclic bridges function as effective magnetic materials. The CPs are created using a variety of techniques (such as hydrothermal, slow evaporation, etc.), and they are then characterized using various spectroscopic techniques (SXRD, TGA, PXRD, FTIR, etc.). The $\pi\cdots\pi$, C-H$\cdots\pi$, and H-bonding processes construct coordination polymers. The Schottky diode is made of materials that have extended π-conjugation, structural flexibility, $\pi\cdots\pi$ interaction, and metal nodes, which are the causes of electrical conductivity in both light and dark conditions. In the study of biology, the CPs are also utilized to extract medications with possible microbiological effects. In ***Chapter 1***, a brief summary and the reasons behind the research are outlined. In ***Chapter 2*** Zn(II)-based 3D CP $\{[Zn_2(tdc)_2(pcih)_2]_n\}$**(1)** ($tdc^{2-}$, 2,5-thiophene dicarboxylate; pich, Pyridine-4-carboxaldehyde isonicotinoyl hydrazine) is structurally characterized by single crystal X-ray crystallography as well as by other spectral data. The material has been used to measure electrical conductivity at dark phase and illumination phase. The anticancer efficiency of **1** has been examined and it shows better impact in inhibiting the proliferation of MDA-MB-231 cells than other cancer cells like HCT-116, HeLa and HepG2. The ***Chapter 3*** reports $\{[Mn_2(tdc)_2(pcih)_2(EtOH)]_n\}$ **(2)**, a 3D supramolecular architecture which shows anti-ferromagnetism. It's interesting to note that the **2**, has electrical conductivity in the semiconducting region. In ***Chapter 4***, a 3D network, $[Zn(mes)(pcih)(H_2O)_2]_n$,**(3)** is constructed by two bridging molecules, mesaconic acid (H_2mes) and pyridine-4-carboxaldehyde iso-nicotinoyl hydrazone (pcih), and shows photoconductivity. In ***Chapter 5*** a 3D-Coordination Polymer of Mn(II), $[Mn_2(aisp)_3(pcih)_2(solvent)]_n$ **(CP1)** (where pcih = Pyridine-4-carboxaldehyde isonicotinoyl hydrazine and H_2aisp = 5-aminoisophthalic acid) which shows both electrical conductivity and anticancer activity against four cancer cell lines (HeLa, PC3, MDA-MB 231, and A549) is reported. The drug delivery activity of Diclofenac Sodium (DMNa) is observed at pH, 7.4 (blood) while at pH, 1.2 (stomach) it remains silent. The ***Chapter 6*** also reports Mn(II)-based CP, $[Mn(tdc)(nvp)_2(H_2O)]\cdot$(DMF) **(Mn-CP)** ($dtc^{2-}$, 2,5-thiophenedicarboxlate and nvp, 4-(1-naphthylvinyl)pyridine) which interestingly shows unique pH-dependent emission [λ_{em}= 525 nm (pH = 2.0-4.0) and 450 nm (pH = 5.0-12.0)]. The emission is quenched by Pd^{2+} in aqueous medium in presence of other thirteen cations with reasonably low pH-dependent limits of detection [21.178 ppb (pH= 3), 15.005 ppb (pH = 7.0) and 59.940 ppb (pH = 10.0)].

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