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ENHANCED SEMICONDUCTING PROPERTIES IN Co-MOF-74 UPON ENCAPSULATION OF ANILINE DERIVATIVES AS GUEST MOLECULES

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Metal-organic frameworks are significant research materials that hybridise organic and inorganic components. The diversified properties like low density, easy tunability, high porosity, and structural properties make MOF a good candidate for the use of semiconductors as well. Among all MOFs, three-dimensional honeycomb-shaped MOF-74, or CPO-27 is unique and forms a one-dimensional hexagonal channel network in which each transition metal ion is bonded to five oxygen atoms. Further, it possesses a specific chemical functionality due to exposed metal sites (EMS), and thereby, MOF-74 records the highest EMS densities among the porous materials but is poor in conductivity. In this study, Co-MOF-74 was synthesized using the room temperature method and tuned up the semiconducting properties by encapsulating -NH_2-containing guest molecules to be applied in solar cell applications. The successful formation of the Co-MOF-74 structure was confirmed using the powder X-ray diffraction data for major diffraction peaks at 6.7° and 11.7° (2θ values) arising from (110) and (300) crystal planes, respectively. According to solid-state UV/Visible data records, the direct band gap for Co-MOF-74 was recorded as 2.72 eV. The Kubelka-Munk equations were used to calculate the band gap energies for different concentrations of aniline and aniline derivatives. The calculated band gap energies were reduced from 2.72 eV to 1.98 eV for the lowest moles of (0.0027 mol) of aniline-encapsulated Co-MOF-74. As the amount of aniline increased to 0.0055 mol and 0.0109 mol, the band gap energies were reduced to 1.96 eV and 1.89 eV, respectively. This trend suggests that there is a potential change in the optical and electronic properties of the material with varying aniline concentrations. Further, the band gap energies for different aromatic amines were determined, and the calculated band gap energies were 1.78 eV, 1.92 eV, 1.89 eV, and 1.87 eV for *o*-anisidine, *p*-anisidine, *m*-toluidine, and *p*-toluidine respectively. According to the Mott-Schottky plot analysis, the Co-MOF-74 exhibits n-type semiconductor behaviour. Additionally, the carrier concentration and flat band potential for varied thickened thin films were found to be 6×10^{20} cm^{-3} (1 µm), 3.68×10^{20} cm^{-3} (3 µm), and -0.48 V (1 µm), -1.00 V (3 µm) respectively. Hence, this study provides evidence of semiconducting property variation upon guest molecule encapsulation.

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Keywords: EMS, Encapsulation, Guest molecules, MOF, Solar cells.