

Progress Seminar

Seminar Title	: β -Ketoenamine based Covalent Organic Frameworks for treating emerging aqueous contaminants and CO ₂ utilisation
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Venue	: Department Library, Department of Chemical Engineering
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Abstract	Covalent organic frameworks (COFs) are crystalline porous polymers that enable the precise incorporation of organic units to form predetermined skeletons and nanopores. They possess a range of distinctive attributes, including the ability to be designed for specific structures and long-lasting durability, significant electron conjugation, the ability to capture light energy, and the quality of being semiconducting which have contributed to their considerable growth in recent years, providing a prospective boost for achieving visible light-induced organic reactions by photocatalysis. In this study, a novel green synthesis was devised to produce a β-Ketoenamine based COF using a deep eutectic solvent. The XRD analysis of the COF was conducted under various reaction circumstances, revealing that a 1:1.5 PTSA DES: H₂O ratio, 24 hours duration, and 120°C constituted the optimal conditions for producing crystalline COF. FTIR study under diverse reaction conditions demonstrated that the requisite bonds of the COF were formed. The COF sample exhibited a C=C bond at 1587 cm⁻¹, attributed to the robust hydrogen bonding in the keto form of the 2D COF framework. The two peaks, C=C at 1464 cm⁻¹ and C-N at 1258 cm⁻¹, correspond to the aromatic C=C and freshly formed C-N bonds in the keto form of the COF structure. The FTIR plots of the COFs indicated the absence of peaks corresponding to the monomers in the synthesized COFs. Yield calculations indicated a high yield of 83.49%. N₂-sorption study revealed a BET surface area of 698.69 m²/g and a BJH pore diameter of 2.8 nm, thereby affirming the mesoporous architecture of the COF. The Raman spectra exhibited all the characteristic shifts of the COF attributed to the C-H, N-H, C-N, and C=C bonds within the COF structure. The full XPS spectra validated the existence of carbon, oxygen, and nitrogen components. High-resolution XPS C1s, O1s and N1s spectra exhibited peaks at 284.1, 285.5, and 287.2 eV, at 530.4, 531.8 eV, 399.7 and 402.4 eV attributable to the C-C, C-N, C=O, C=O and C-O-H, C-N bond and π-π^* transition of COF. The FESEM pictures of COF-120 exhibited a complex cross-linked fibrous network interlinked by wire-like structures due to robust π-π stacking interactions among neighbouring rods. High-Resolution Transmission Electron Microscopy (HRTEM) revealed analogous cross-linking structures. The SAED pattern validated the polycrystalline characteristics of the COF. The UV-Vis DRS spectra indicated that the synthesized COF sample exhibits a broad absorption band over the UV and visible light spectrum, with an absorption edge at 625 nm, demonstrating the material's activity under visible light. The K-M plot confirmed that the material's band gap is 2.14 eV. The PL spectra exhibited a wide absorption band about 630 nm, likely resulting from the extensive π-π stacking of the COF. The preliminary photocatalytic degradation investigation revealed that under optimal conditions of 10 mg catalyst dose and 5 ppm sulfamethazine concentration, 93.2% of sulfamethazine was degraded within 120 minutes of visible light irradiation.