**ABSTRACT**

The present work is focused on fundamental understanding of different properties of metal organic framework (MOF) and its composites, applied towards catalytic and adsorptive remediation of contaminated water.

The excellent potentials of MIL-88A(Fe)/$MoS_2$, MIL-100(Fe)/$Bi_2S_3$, MIL-53(Fe/Co)/$CeO_2$, MIL-53(Fe/Co)/$MoS_2$ and ZIF-67/gCN were explored towards UV/Visible light driven photocatalytic degradation of Bisphenol-A (BPA), Rhodamine-B (RhB), Atrazine (ATZ) and Sulfamethoxazole (SMX), in presence of Peroxymonosulfate (PMS) activation, and catalytic reduction of p-Nitrophenol (PNP) in aqueous medium, respectively. (0.01-0.1) g/L catalyst and (0.15-0.5) g/L PMS could degrade (98.2-99.9)% organic contaminants (with ≥75% mineralization), within 30-60 min of UV/Vis light exposure. For each case, effects of various coexisting ions and organics on the degradation process were investigated. Solvo/hydrothermal and coprecipitation based synthesis methods were used to prepare the MOFs and resultant binary composites. The coprecipitation based synthesis, for the synthesis of ZIF-8 and ZIF-67/gCN, is a green and aqueous based method, without any thermal or mechanical energy input. Radical scavenging and EPR analysis were employed to identify the various reactive species in the medium and corresponding contributions from radical and non-radical based mechanisms. The importance of various surface-bound redox cycles, i.e., $Fe^{2+}/Fe^{3+}\big|_{surf.}$, $Co^{2+}/Co^{3+}\big|_{surf.}$ $Bi^{3+}/Bi^{4+}\big|_{surf.}$, $Ce^{3+}/Ce^{4+}\big|_{surf.}$ and $Mo^{4+}/Mo^{6+}\big|_{surf.}$ towards PMS activation and reactive species generation was studied in details. On the other hand, 0.15 g/L ZIF-CN(5) and 0.35 g/L $NaBH_4$ could completely reduce PNP, within 5 min of UV exposure. For all these catalytic studies, the generated intermediates and by-products were identified using LCMS/MS and MALDI-TOF/MS analysis.

Porous ZIF-8 MOF was employed as a suitable adsorbent for heavy metals, i.e., Pb and Cd, from synthetic and real-life battery effluent. The ZIF-8 powder was embedded inside porous polymeric matrix to prepare macrosized mixed matrix polymeric beads (MMBs) which were further used as suitable adsorbent media in adsorption columns. The macrosized beads were synthesized through a facile, phase-inversion based technique using water as the antisolvent. Solidification of the

polymeric matrix with dispersed MOF particles generate porous and mechanically stable adsorbent. The maximum adsorption capacities of the MMBs were estimated as 220 mg/g for Pb and 161 mg/g for Cd, respectively, at pH of 6.5 and temperature 298K. Long-duration column run studies were conducted to determine the effects of various parameters, namely, inlet flow rate, feed concentration and column height, and corresponding scaleup performance was predicted from the pore diffusion-adsorption based transport model.

**Keywords**: *Metal organic framework (MOF); Heterojunction photocatalyst; Mixed matrix beads; Catalytic degradation, Adsorption; Peroxymonosulfate; Bisphenol-A; Atrazine; Sulfamethoxazole; Rhodamine-B; Nitrophenol; Heavy metals.*