Indian Institute of Technology Delhi

School of Interdisciplinary Research (SIRe)

SIRe Project Number

2024-02-32

Project Proposal for Ph.D.

Project Details	
Project Title	Robust and porous amino acid-functionalized metal-organic frameworks for effective removal of heavy metals from water
Project Summary (Minimum 500 and maximum 2000 characters)	We propose to synthesize isoreticular amino acid-functionalized MOFs with different pore sizes for adsorption of heavy metals in water. A library of amino acid-functionalized MOFs will be synthesized via post-synthetic grafting of easily affordable amine-tagged zirconium UiO-MOFs. UiO-type MOFs built from $Zr_6(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_4$ SBUs and linear dicarboxylate linkers are highly robust under wide range of pH in aqueous medium. The tandem amide coupling between the amino-group of MOF and the carboxylic acid group of N-Fmoc-protected amino acid in the presence of HBTU and diisopropylethylamine, and subsequent deprotection of amino-group would afford amino acid-grafted UiO-MOFs. Using the similar method, mixed amino acid functionalized MOFs will also be prepared. The adsorption properties of MOFs will be optimized by varying the pore sizes and also by changing the ratio of the different amino acids grafted within MOFs. The MOFs will be characterized by XRD, TGA, XPS, SEM, TEM, FTIR, BET and NMR. The adsorption capacity of MOF will be evaluated by conducting kinetics and isotherm studies using in single and multicomponent solutions of heavy metals. Chromium, lead, zinc, arsenic and copper will be selected for the present study. The concentrations of these metals will be analyzed by ICP-MS. Studies on regeneration and reuse potential of MOF will be conducted and a suitable (thermal or chemical) regeneration method will be selected. In real water or wastewater matrix, there will be interferences or other competing or inhibiting substances. Hence the effect of factors such as pH, conductivity and the presence of other multivalent cations will be evaluated. For practical applications, the MOF will be coated on membranes or pelletized using polymers and using lab scale set up the performance of the treatment unit will be evaluated under different operating conditions. Based on the results of lab studies, a strategy for upscaling will be proposed for field scale implementation. **<u>Interdisciplinary Nature of the Project:</u>** Dr. Manna has broad experience in developing porous MOFs for catalysis and gas adsorption. His expertise in synthetic chemistry will aid in preparing amino acid-functionalized MOF, and also will contribute in tuning and modifying the functionalities of MOFs to meet the requirement. Dr. Arya has expertise in performance evaluation of water and wastewater treatment technologies and will contribute to the experimental studies on MOF to develop modular water treatment unit to be implemented in field.

Ph.D. Supervisors			
Role	**Name of Faculty**	**Academic Unit in IITD/Institute/University**	**Email ID (Official)**
Supervisor 1	Prof. Arya V	Civil Engineering (IITD)	aryav@iitd.ac.in
Supervisor 2	Prof. Kuntal Manna	Department of Chemistry (IITD)	kmanna@chemistry.iitd.ac.in

Project requirements (Student qualifications, experience required, etc)
***The candidate will be shortlisted based on common shortlisting criteria decided by ScRC (SIRe)**

- M.Sc in Chemistry/Environmental Science with a valid NET score/JRF fellowship

Source of fellowship/funding
(CSIR/UGC/DBT/ICMR/ICAR/NEET-PG/DST-INSPIRE/IRD/FITT Project details, if any)

Candidate with his/her own fellowship/ Institute Fellowship

Role of Faculty Members involved:	
Supervisor-1	In Dr Arya's lab: • Test the potential of MOF for the removal of heavy metals from water. • study adsorption kinetics and optimize the adsorption parameters by fixed bed column or MOF coated membrane. • The design and upscaling scheme for field implementation will also be conducted in Dr Arya's lab.
Supervisor-2	In Dr. Manna's lab: • The synthesis and characterization of amino acid-functionalized MOFs. • Investigate the stability of MOFs in aqueous medium as well as its regeneration potential.