Poster Presentation

Design of Zn(II)-MOF for Selective Aqueous phase Sensing of TNP

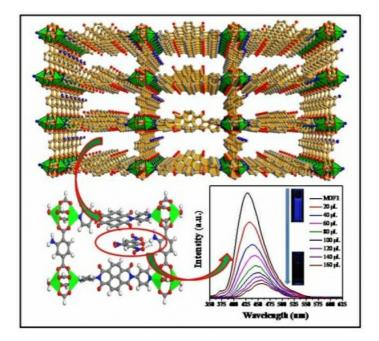
<u>Nayuesh Sharma</u>¹, C. M. Nagaraja¹ ¹Department of Chemistry, Iit Ropar, Rupnagar, India E-mail: nayuesh.sharma@iitrpr.ac.in

Metal-organic frameworks (MOFs) have emerged as an important class of porous crystalline materials in the last few decades due to their intriguing network topologies and novel properties.[1] A suitable choice of metal ions and organic ligands/linkers play an important role in directing the rational design of MOF materials with high surface areas and tunable pore size for various applications.[2] In this regard, the combination of porosity and luminescence results in MOFs with potential applications for sensing including nitroexplosives. However, the development of luminescent MOF materials by incorporating functional sites to the framework has attracted the researchers due to their improved sensing ability. Among the various nitroexplosives, 2,4,6-trinitrophenol (TNP), has the highest explosive power and has been identified as a toxic pollutant in aqueous medium.[3] Therefore its selective detection in aqueous medium is important for civilian safety. In this context, we developed a 2 -fold Interpenetrated 3D framework of Zn(II) [Zn2(NH2-BDC)2(dpNDI)]n(MOF1), which exhibits highly selective and sensitive detection of TNP in water through luminescence quenching mechanism. The high luminescence quenching of TNP for MOF1 has been attributed to stronger interaction of TNP with the -NH2 group decorated in the pore channels of MOF1 revealed from DFT calculations. The synthesis, characterization and sensing property of MOF1 will be presented.

[1] Yaghi, O. M. et.al. (2003) Nature 423, 705-714.

[2] Deenadayalan, M. S et al. (2016) Inorg. Chem. 55, 5320-5327.

[3] Singh, D. et al. (2015) Cryst. Growth Des. 15, 3356-3365.



Keywords: Metal-organic frameworks, nitroexplosives, selective sensing