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Mechanistic Insights into Metal–Organic Frameworks (MOFs) for Environmental Remediation

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Introduction

- A clean and balanced environment is a precondition to support life on Earth. However, rapid industrialization, agricultural development, and other anthropogenic activities, including improper waste management, resource depletion, and more, result in environmental deterioration.
- Metal–Organic Frameworks (MOFs), the ultimate sustainable approach for environmental remediation possess properties like ultra-high levels of porosity, large internal surface areas (500 -7000 m^2/g), sensitivity, selectivity and more.
- Structural arrangements of the components affect the porous nature of MOFs, and their pore size is also tailored by taking different combinations of organic linkers and metal ions or clusters.
- This paper aims to highlight the various mechanistic pathways including adsorption, photocatalysis, membrane and composite-based mechanisms, and ion-exchange process used for removal of pollutants (heavy metals, synthetic dyes, pesticides, pharmaceutical residues, and also greenhouse gases) and also covers the remediation of air, water and soil (Fig.1,2).
- Nowadays, researchers exploring MOFs as next-generation materials to address the current environmental challenges across the globe.

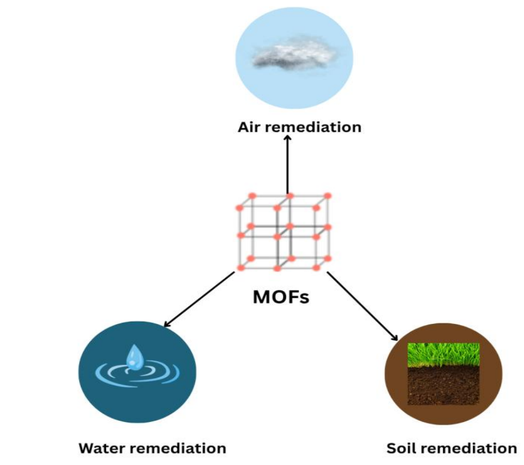

Fig. 1 MOFs in environmental remediation

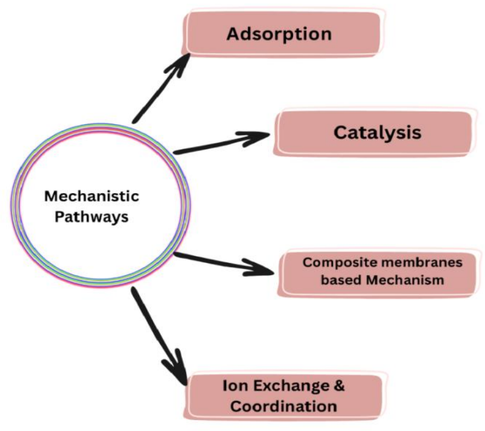

Fig. 2 Mechanistic pathways for removal of pollutants

Mechanistic Pathways in Environmental Remediation by MOFs

❑ Adsorption:

- As adsorbents, MOFs represents a sustainable category that control pollution via surface phenomenon called adsorption.
- High structural stability , selectivity and great adsorption capacity are the major features that makes them good adsorbent.
- A single adsorbate molecule may carry out more than one process like Cr (VI) adsorbate adsorb on $Ni_{0.6}Fe_{2.4}O_4$-UiO-66-PEI using variety of electrostatic attraction, chelation, and even a redox reaction.

❑ Catalytic Mechanisms

- Catalysis, a solar-powered green degradation process, has enormous potential for pollutant degradation.
- This mechanism initiated by absorption of light which leads to charge transfer usually from ligand to metal centre and results in generation of electrons and holes.
- So, species like O_2, H_2O etc. accept the photogenerated electrons and holes that give various reactive oxygen species (ROS) like $\bullet O_2^-$ and •OH respectively, which then attack on pollutants (Fig. 3).

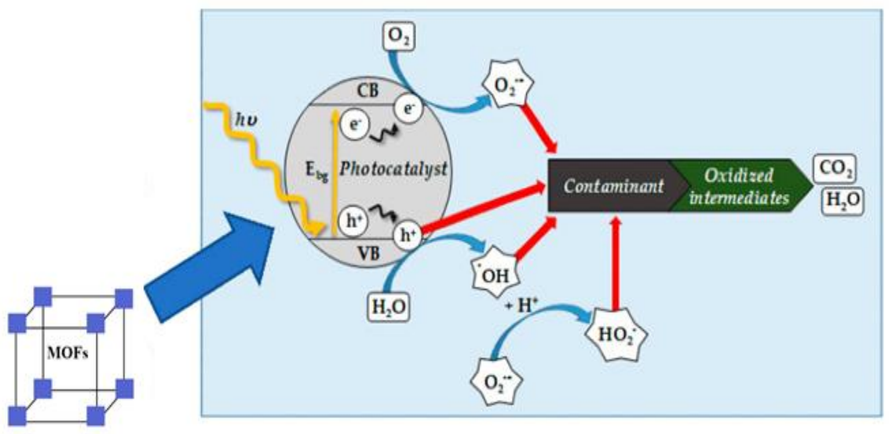

Fig. 3 Photocatalytic degradation mechanism

- The photocatalytic degradation of organic dyes like methylene blue, using Ni-Co/NC is more efficient than Co/NC and Ni/NC.
- Bimetallic frameworks are more efficient than frameworks containing one type of metal centers.

❑ Ion-Exchange & Coordination:

- Ion exchange involves the replacement of metal ions as SBUs or metal nodes and the counter ions present within the pores or channels to neutralize the excess charge of the framework.
- This mechanism is completely reversible that retains the basic composition of MOFs.

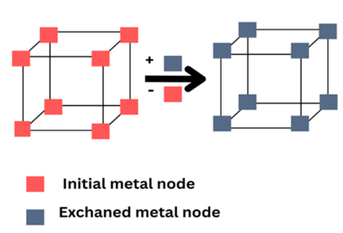

Fig. 4 Ion-exchange at metal node (Cationic)

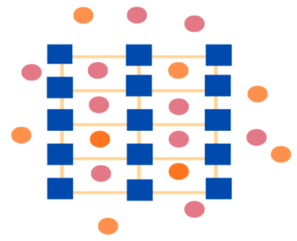

Fig. 5 Ion-exchange through pores (Anionic)

- (MIL-101(Cr)-Cl) is achieved by exchanging F^- in pristine MIL-101(Cr) through anionic mechanism that is more effective to remove 2,4-dichlorophenoxyacetic acid (2,4-D) from water (Fig. 4,5).

❑ Membrane and Composite-based Mechanisms:

- This mechanistic pathway has been reported with tremendous degradation ability for pollutants like dyes and antibiotics.
- The separation performance of MOF-74(Ni)@GO composites and Pebax®1657-MOF-74(Ni)@GO membranes is more compared to pristine MOF-74(Ni) considering that graphene oxide must be completely dispersed.

MOFs in Environmental Applications

❑ Air remediation:

- Unique characteristics of MOFs allow them to effectively capture and remove varied airborne contaminants, such as volatile organic compounds (VOCs), toxic industrial gases (NH_3, SO_2, and NO_x), and greenhouse gases such as CO_2 (Fig. 6).
- MOF-199 and MIL-101(Cr) show uptake of VOCs like benzene due to formation of strong π-interactions while Co_2Cl_2BBTA and Co_2Cl_2BTDD are the two cobalt based MOFs that exhibits strong affinities toward ammonia (NH_3).

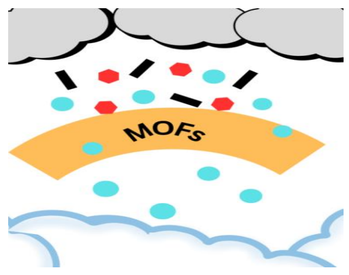

Fig. 6 MOFs in air-remediation

❑ Water remediation:

- MOFs presents a highly promising class of materials that are helpful in removing pollutants from water effectively.
- These materials are stable in water under varying temperature, pH, and humidity.
- The Zn(BDC)-MOF exhibits excellent adsorption behavior toward both methylene blue and aniline blue, irrespective of their opposite ionic charges.
- Fe_3O_4@AMCA-MIL53(Al) possess the ability to adsorb radioactive metals U(VI), Th(IV).

❑ Soil remediation:

- Pesticides (DDT and chlorobenzenes) are persistent organic pollutants that remain in soil and the untreated wastewater containing heavy metals, polycyclic aromatic hydrocarbons (PAHs), aromatic compounds, etc. when released from industries in water results in soil contamination.
- ZIF-8 and ZIF-67 are the two MOFs that show high adsorption for both ethion and prothiofos (pesticides).

Conclusion

- This work emphasise the importance of MOFs to overcome the current environmental issues that have great potential for the adsorption and elimination of hazardous contaminants present in air, water, and soil.
- Structural aspects of these frameworks decide the mechanistic approach for a variety of pollutants. Additionally, we conclude that modifications to these frameworks show great influence over their performance.

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