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Functionalized MOFs for Selective Dye Removal: A Mechanistic Study of Cationic and

Anionic Adsorption

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INTRODUCTION

- Industrial effluents from textile and dye industries release toxic dyes, causing severe environmental pollution.
- Conventional treatment methods often fail to remove these dyes completely due to their chemical stability and complex structures.
- Metal-Organic Frameworks (MOFs) are porous crystalline materials with high surface area and tunable pore structures, making them promising adsorbents.
- Functionalization of MOFs enhances selectivity toward cationic or anionic dyes.
- Adsorption occurs through multiple mechanisms: electrostatic interactions, π – π stacking, hydrogen bonding, and pore confinement.
- This study explores the mechanistic aspects of dye adsorption by functionalized MOFs to understand structure—property relationships.
- Insights gained will aid in designing efficient, selective, and sustainable MOF-based materials for wastewater purification.

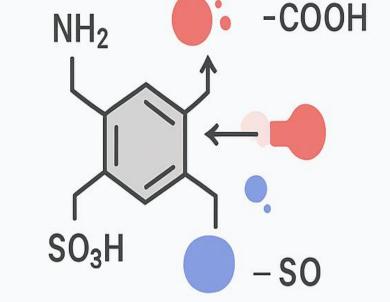
FUNCTIONALIZATION OF MOFS

Metal-Organic Frameworks (MOFs)

are porous hybrid materials composed of metal nodes and organic linkers.

Types of Functionalization

1. Pre-synthetic functionalization:
Functional groups (-NH₂, -COOH, -OH, SH, etc), and organic linkers before MOF synthesis.



2. Post-synthetic modification (PSM):

Chemical modification of pre-formed MOFs without disrupting their structure.

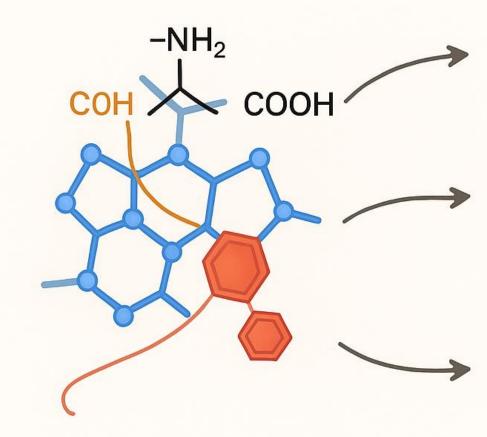
Role in Dye Adsorption

- Functional groups influence surface charge, polarity, and pore environment, determining interactions with dye molecules or molecules.
- Cationic dye adsorption: Favored by negatively charged or ipnonont pointed functional groups, inna inurace arttraction, and pore confinement.

CONCLUSION

Functionalized MOFs exhibit selective adsorption of cationic and anionic dyes through tailored surface charges and functional groups. Electrostatic interactions, hydrogen bonding, and π – π stacking govern the adsorption mechanism, making these MOFs efficient and tunable materials for water purification and dye removal applications.

Mechanism of Dye Adsorption in Functionalized MOFs

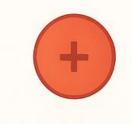


Overall Insight

Synergistic effects of electrostatic, π – π and hydrogen-bond interactions determine dye selectivity and capacity.

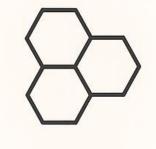
Electrostatic Interaction

Major driving force between charged dye molecules and oppositely charged MOF surfaces



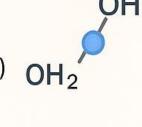
π – π Stacking Interaction

Occurs between aromatic rings f dyes and organic linkers in MOFs Enhances adsorption of dyes with conjugated aromatic struct-



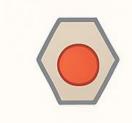
Hydrogen Bonding

Formed between dye moleiles and functional groups (-OH₄-NH₂-COOH) OH₂ on MOF surfaces, Stabilizes dye molecules within pores



Pore Confinement Effect

Dyes are physically trapped within MOF pores due to size compatibility Enhances adsorption capacity



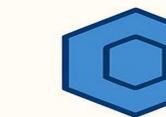
CATIONIC VS. ANIONIC DYE ADSORPTION

Dye Type & Charge

Favorable MOF Surface



Cationic dyes



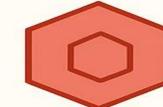
-coo-

-SO₃-



Anionic dyes (e.g. MO, CR)

(e.g. MB, RhB)



-NH₃⁺

Key Interaction

Electrostatic + H-bonding + π-\t



Funcuational groups → selective dye adsorption



pH tuning → control MOF surface charge & selectivity



Efficient for water purification & dye separation

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