

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

Priya Mishra, Satya, Kulsum Hashmi, Armeen Siddique, Seema Joshi*
Department of Chemistry, Isabella Thoburn College, Lucknow, UP 226007, India

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:

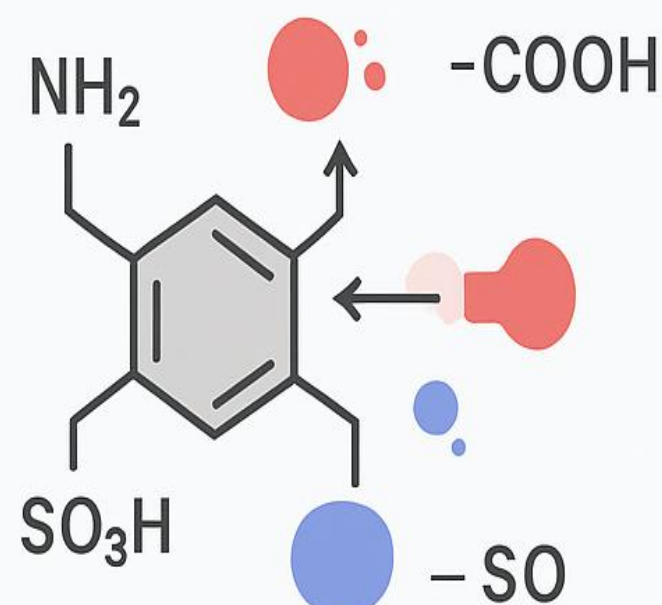
Functional groups ($-\text{NH}_2$, $-\text{COOH}$, $-\text{OH}$, SH , etc), and organic linkers before MOF synthesis.

2. Post-synthetic modification (PSM):

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

Role in Dye Adsorption

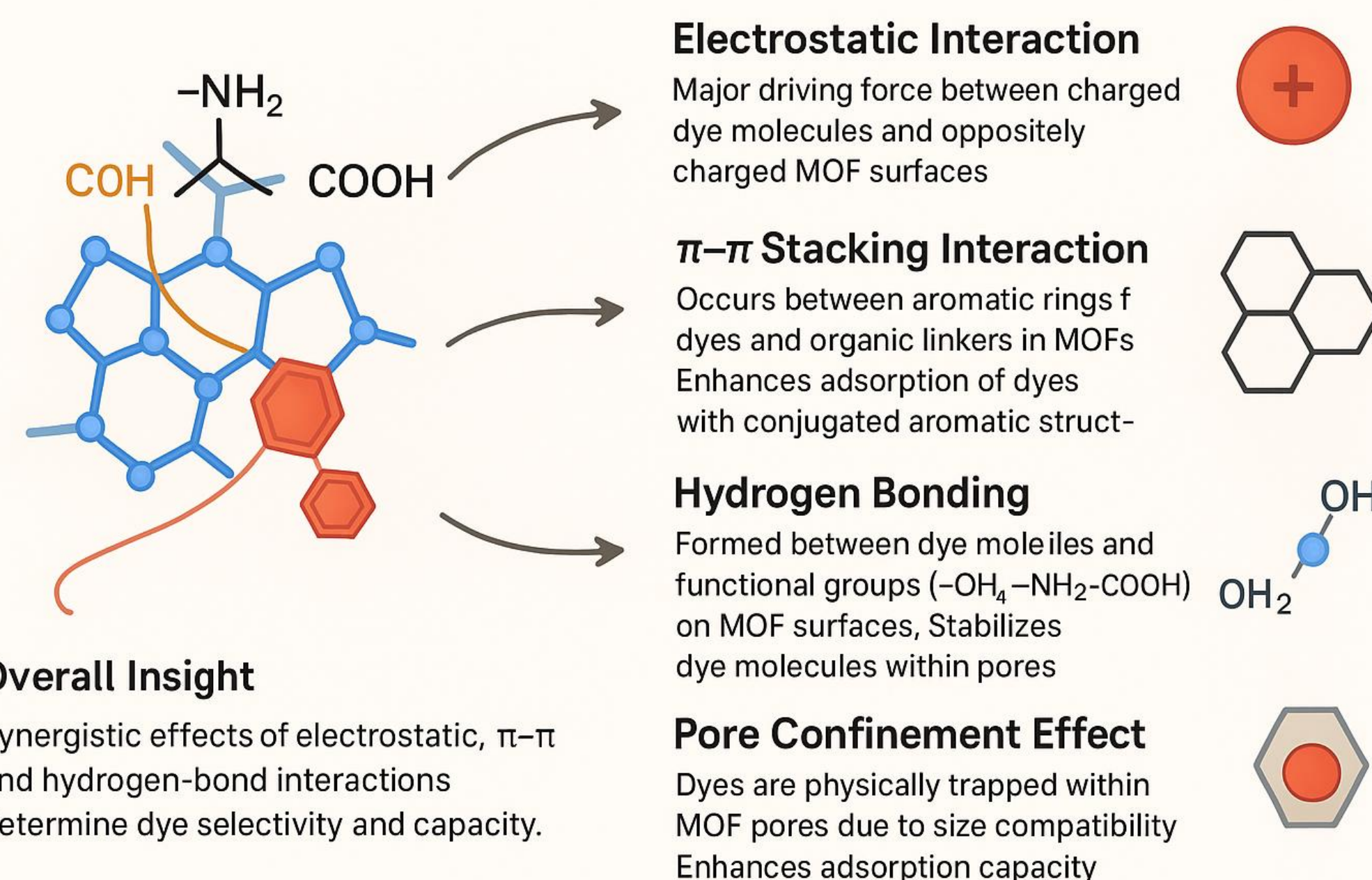
- Functional groups influence **surface charge**, **polarity**, and **pore environment**, determining interactions with dye molecules or molecules.
- Cationic dye adsorption:** Favored by negatively charged or nonpolar functional groups, intramolecular attraction, and pore confinement.



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

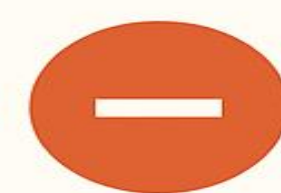


CATIONIC VS. ANIONIC DYE ADSORPTION

Dye Type & Charge

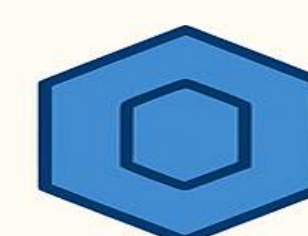


Cationic dyes
(e.g. MB, RhB)

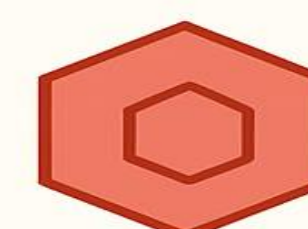


Anionic dyes
(e.g. MO, CR)

Favorable MOF Surface



$-\text{COO}^-$
 $-\text{SO}_3^-$



$-\text{NH}_3^+$
 $-\text{OH}^+$

Key Interaction

Electrostatic + H-bonding + π – π



Functional groups → selective dye adsorption



pH tuning → control MOF surface charge & selectivity



Efficient for water purification & dye separation

REFERENCES

- [1] Li, J.-R., Sculley, J., & Zhou, H.-C. Chem. Rev., 2012, 112, 869–932.
- [2] Hasan, Z., & Jung, S. H. J. Hazard. Mater., 2015, 283, 329–339.
- [3] Wadhawan, S., Sharma, S., & Singh, K. Coord. Chem. Rev., 2021, 436, 213777.
- [4] Dhaka, S., Kumar, R., Deep, A., & Kurade, M. B. Coord. Chem. Rev., 2019, 380, 330–352.
- [5] Fang, Q., & Guo, H. Adv. Mater., 2020, 32, 2001942.