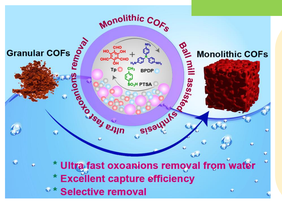
Disorder Driven Triphenylamine Based Monolithic Covalent Organic Framework for the Efficient Removal of Toxic Oxo-Anions From Water

Arjun Warrier, Pampa Jhariat and Tamas Panda*
Department of Chemistry, Vellore Institute of Technology(VIT), Vellore, Tamil Nadu, India.
Email-arjun.warrier4539@gmail.com

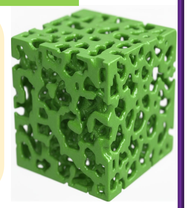
6th Commonwealth Chemistry Posters
Building Networks to Address the Goals
1-2 October 2025

Introduction

Why Monolithic COFs?



- *Hierarchical structure*
- *Easy handling*
- *Structural flexibility*
- *High chemical Stability*
- *High Mechanical Stability*



Higher adsorption capacity → **Accelerated adsorption kinetics** → **Bridge Gap between COF and Practical application**

Motivation and Design Strategy

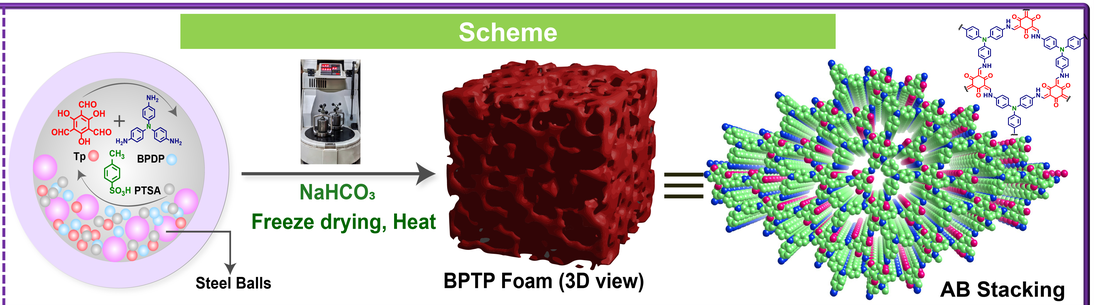
Advantages of Triphenyl Amine

- **Electron-donating group**
- **Conjugated π-system.**
- **Electron rich aromatic ring-can interact**
- **Can interact with pollutant through π–π stacking and electrostatic interactions.**

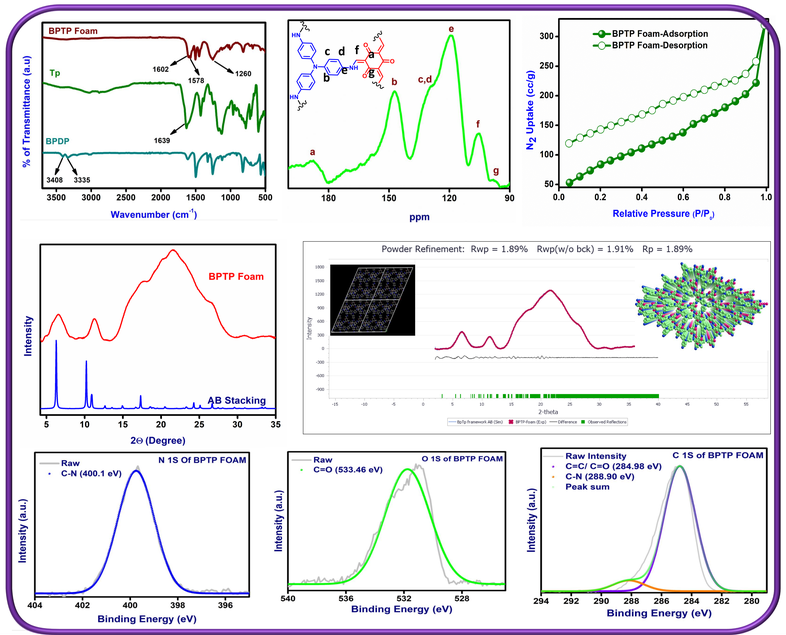
Objective

- *Develop monolithic COFs using industrially friendly methods to enable scalable, binder-free, and mechanically robust adsorbents.*
- *Introduce hierarchical porosity (micro–meso–macropores) for improved mass transport and accelerated diffusion kinetics.*
- *Design neutral COFs with tailored electrostatic interactions to enhance selective adsorption and minimize secondary contamination.*

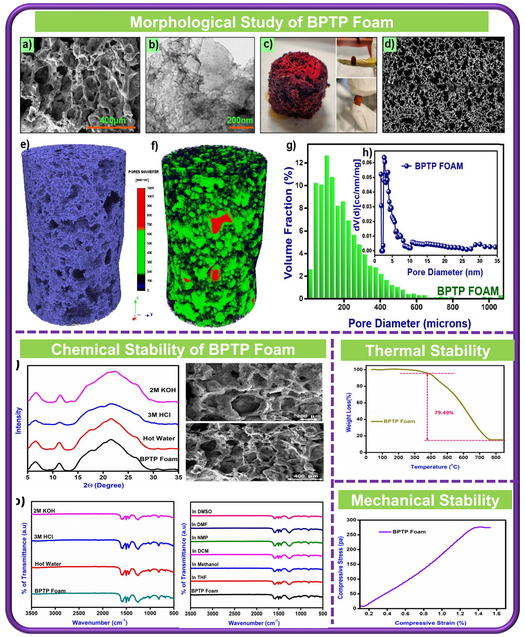
Scheme



Characterization of BPTP Foam



Morphological Study of BPTP Foam



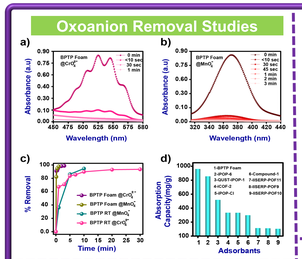
Chemical Stability of BPTP Foam

Thermal Stability

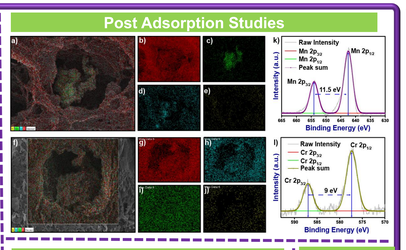
Mechanical Stability

Adsorption Studies Using BPTP Foam

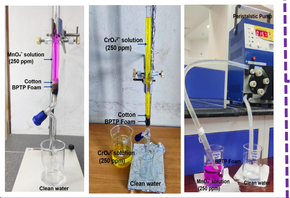
Oxoanion Removal Studies



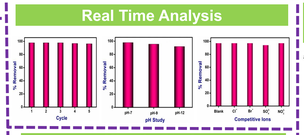
Post Adsorption Studies



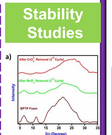
Real Time Application



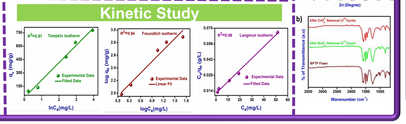
Real Time Analysis



Stability Studies

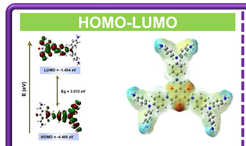


Kinetic Study

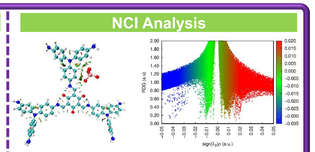


Theoretical Studies

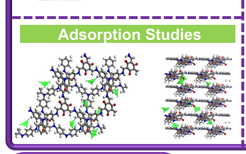
HOMO-LUMO

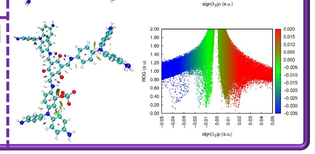


NCI Analysis

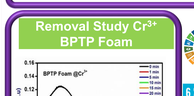


Adsorption Studies





Removal Study Cr^{3+} BPTP Foam



Conclusion

- ***Simple, scalable synthesis:*** We report an industrial-friendly, ball mill-assisted in-situ gas-forming route to a monolithic, hierarchically porous BPTP Foam (one-pot, green, easily scalable)
- ***Hierarchical structure & robustness:*** The foam exhibits Interconnected micro–meso–macroporosity with high structural and chemical stability.
- ***Outstanding adsorption performance:*** MnO_4^- Q_{ads} = **961.54 mg·g^{-1}** (complete removal = **1 min**) and CrO_4^{2-} Q_{ads} = **448.09 mg·g^{-1}** (≈ **3 min**), placing BPTP Foam among the highest performing porous sorbents reported.
- ***Fast kinetics & high affinity:*** Rapid pseudo-second-order uptake withvery large distribution coefficients (high Kd values) and excellent selectivity for oxo-anions even in the presence of competing anions (Cl^-, NO_3^-, SO_4^{2-}, Br^-).
- **Reusability & practical operation:** Column studies and regeneration (acid wash) show **~94–95%** capture efficiency retained after multiple cycles; demonstrated column/pump operation for continuous removal.
- ***DFT and RDG analyses*** indicate strong non-covalent interactions (H bonding / π interactions) between the oxo-anion oxygen atoms and triphenylamine moieties; MnO_4^- shows the strongest binding; explaining superior capacity and kinetics.
- ***Monolithic form avoids secondary contamination and tedious separation associated with powders, lowers operational complexity, and reduces costs ; facilitating translation to large-scale water remediation.***
- **This work provides** a direct contribution to ***SDG 6 (Clean Water and Sanitation)*** by enabling rapid, selective removal of toxic oxo-anions from water.
- **This work provides** an advance toward ***SDG 9 (Industry, Innovation & Infrastructure)*** through a mechanochemical, scalable, one-pot synthesis suited to industrial production

References

1. **Warrier, A.**; Jhariat, P; Vergese, M.; Panda, P.; Panda, T.*, *Small* 2025, Accepted Manuscript. DOI 10.1002/smll.202506837 (**This Work**).
2. Panda, T.; **Warrier, A**; Jhariat, P.; Varghese, M.; Hierarchical Porous Monolithic Covalent Organic Framework for the Removal of toxic Oxoanions from Water and Applications Thereof. ***(Published; Application no- 202541053981, Indian Patent)***
3. Jhariat, P.; **Warrier, A.;** Vergese M.; and Panda, T.*, *J. Mater. Chem. A* 2025, **Accepted Manuscript. DOI-** https://doi.org/10.1039/D5TA01161B

Acknowledgment

Advanced Porous Materials Lab