# Molecular-level Design Strategy in 2D-Organic Frameworks for Efficient Desalination and Resource Recovery

**Dinesh Shetty**[1, 2]
Najat Maher Aldaqqa,[1] Rajesh Dhanushkoti,[1] Sushil Kumar[1] José I Martínez[3]
[1]*Khalifa University, Abu Dhabi, 127788, UAE*
[2]*Center for Catalysis & Separations (CeCaS), Khalifa University, Abu Dhabi, 127788, UAE*
[3]*Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain*

dinesh.shetty@ku.ac.ae

Abstract (Arial 10)

Capacitive deionization (CDI) has emerged as a transformative, energy-effective, and cost-effective solution for sustainable desalination technology, offering fresh water from brackish. Hybrid CDI (HCDI), which operates via a faradic storage mechanism is considered the next generation of CDI due to its superior desalination capacity and charge efficiency.[1] However, the current system suffers from a low desalination rate and short-term stability, primarily due to inefficient charge transfer, restricted ion transport, and structural instability.[2, 3] HCDI can also be used for resource recovery from brine and/or wastewater. In both applications of HCDI, the molecular-level design of electrode materials plays a crucial role.[4] To tackle these challenges, we have been working on rationally designing 2D-organic framework materials by utilizing their structural and functional tunability. Our findings revealed a remarkable chloride ion removal capacity (Cl-RC) of 71.5 mg g–1 in 1300 ppm saline solution with a noteworthy removal capacity rate (Cl– RCR) of 1.85 mg g–1 min–1.[5] Also, we have a series of materials showing highly selective (>99%) recovery of Li from brine with excellent efficiency.[6] The talk will focus on design principles and performance metrics of novel electrode materials developed in my group.

## References

[1] Mauter, M. S. et al. The role of nanotechnology in tackling global water challenges. *Nat. Sustain*. 1, 166–175 (**2018**).
[2] Sun, K. *et al.* Electrocapacitive Deionization: Mechanisms, Electrodes, and Cell Designs. *Adv. Funct. Mater.* 33, 2213578 (**2023**).
[3] Gamaethiralalage, J. G. et al. Recent advances in ion selectivity with capacitive deionization. *Energy Environ. Sci.* 14, 1095–1120 (**2021**).
[4] Kumar, S., Aldaqqa, N. M., Alhseinat, E. & **Shetty, D***. Electrode Materials for Desalination of Water via Capacitive Deionization. *Angew. Chem. Int. Ed*. 62, e202302180 (**2023**).
[5] Aldaqqa, N. M., Kumar, S., Martinez, J. I., Elmerhi, N., Alhseinat, E. & **Shetty, D*** Surface Engineered 2D-β-ketoenamine Covalent Organic Framework for Superior Dechlorination via Hybrid Capacitive Deionization, *Angew. Chem. Int. Ed*. 137 (37), e202510345 (**2025**).
[6] Dhanushkotti, R., Mohammed, A. K., Ranjeesh, K. C., Krishnegowda, H. M., Aldaqqa, N. M. & **Shetty, D***. Inherited Nitrogen Distribution Control in Covalent Organic Framework Cathodes for Efficient Electrochemical Lithium Recovery via Capacitive Deionization, *Adv. Sci. 2417140 (**2025**)*

## Figures

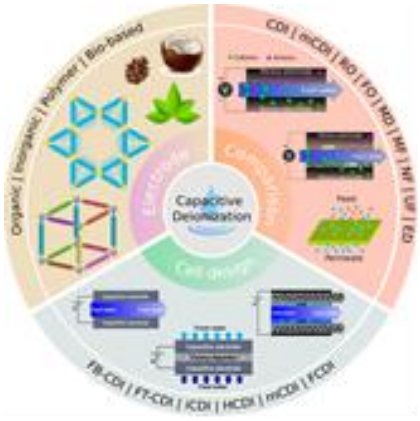


**Figure 1:** Novel strategy to develop 2D-organic framework electrode materials for efficient desalination.