S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Chemical and Biological Sciences

06th January 2026 **4.00 PM** **ONLINE / FERMION**

SPEAKER

Dr. Soumya Mukherjee,
Associate Professor of Materials Chemistry in the Dept. of Chemical Sciences
at the University of Limerick (UL)

TITLE OF THE TALK

Environmental Systems and Sustainable Structural Adaptiveness-enabled High Selectivity in Transiently Porous Crystals Development: An Editorial Perspective

ABSTRACT

Our recent results (published and ongoing studies) on the crystal engineering of several classes of transiently porous and ultramicroporous (pore size < 7 Å) porous crystals will be our focus. 1 Guest transport through discrete voids (closed pores) in crystalline solids is poorly understood. In 2025, we reported a transiently porous azolate coordination network (ACN), featuring square lattice (sql) topology and the bent linker 1,3-bis(1H-imidazol-1-yl)benzene. [2] Albeit crystallographically identifying the absence of a permanent guest transport pathway, this ACN was found to undergo phase transformations between distinct closed pore phases in response to desolvation, humidity, and/or exposure to CO2 and C2 H2 gases. Investigating its guest transport mechanism, we uncovered a crystal engineering strategy with potential to enable the design of transient porosity in similar compounds. In 2025, drawing on a comparison of two propyne (C3H 4)-selective and propylene (C3 H6)-rejecting porous molecular crystals of cyclotetrabenzoin and its tetraacetate derivative, and using a combination of in situ synchrotron powder X-ray diffraction and molecular dynamic simulations, we established how peristaltic motion facilitates light hydrocarbon transport, but erodes selectivity.[3] This work breaks new ground on emphasising the importance of often subtle structural adaptations in sorbent structures to the dynamic column breakthrough separation performances, and offers a new design strategy (Fig. 1) for gas sorption in transiently porous and ultramicroporous sorbents. [Detailed in page -2]

HOST FACULTY

Dr. Pradip S Pachfule, Associate Professor

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Structural Adaptiveness-enabled High Selectivity in Transiently Porous Crystals

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Our recent results (published and ongoing studies) on the crystal engineering of several classes of transiently porous and ultramicroporous (pore size < 7 Å) porous crystals will be our focus.[1] Guest transport through discrete voids (closed pores) in crystalline solids is poorly understood. In 2025, we reported a transiently porous azolate coordination network (ACN), featuring square lattice (**sql**) topology and the bent linker 1,3-bis(1*H*-imidazol-1-yl)benzene.[2] Albeit crystallographically identifying the absence of a permanent guest transport pathway, this ACN was found to undergo phase transformations between distinct closed pore phases in response to desolvation, humidity, and/or exposure to CO_2 and C_2H_2 gases. Investigating its guest transport mechanism, we uncovered a crystal engineering strategy with potential to enable the design of transient porosity in similar compounds. In 2025, drawing on a comparison of two propyne (C_3H_4)-selective and propylene (C_3H_6)-rejecting porous molecular crystals of cyclotetrabenzoin and its tetraacetate derivative, and using a combination of *in situ* synchrotron powder X-ray diffraction and molecular dynamic simulations, we established how *peristaltic motion* facilitates light hydrocarbon transport, but erodes selectivity.[3] This work breaks new ground on emphasising the importance of often subtle structural adaptations in sorbent structures to the dynamic column breakthrough separation performances, and offers a new design strategy (**Fig. 1**) for gas sorption in transiently porous and ultramicroporous sorbents.

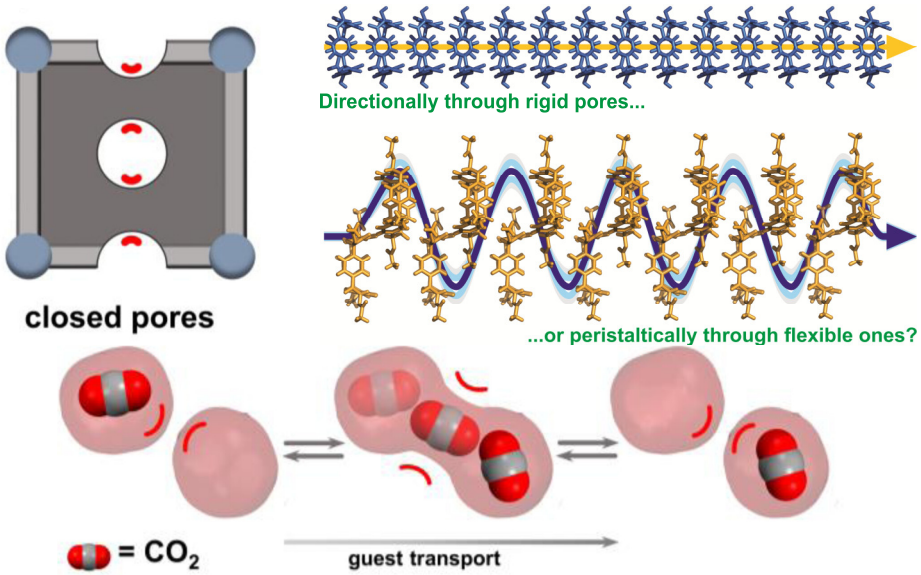

Fig. 1: Porosity "*without pores*": a crystal engineering strategy to enable the design of transient porosity in underexplored reticular sorbents, *e.g.*, by *peristaltic* motion of structurally adaptive porous crystals.

References

[1] X. Li, S. Mukherjee*, and M. J. Zaworotko*, *Adv. Mater.*, just accepted (2025); [2] K. Koupepidou, *et al.*, *Angew. Chem. Int. Ed.*, *64*, e202423521 (2025); [3] Y.-H. Lin, *et al.*, *J. Am. Chem. Soc.*, *147*, 43957 (2025).

CV of the Speaker

Prof. Soumya Mukherjee (SM) is an Associate Professor of Materials Chemistry in the Department of Chemical Sciences at University of Limerick (UL). His recent recognitions include the UL President's Research Output Award (2025), UL President's Research Output Award – Consolidator (2025), Thieme Chemistry Journals Award (2025), and the Research Ireland–Wales Innovation Network Research Alliance Award (2025). In 2024, SM received the Bernal Institute Mid-Career Researcher Award, the SSPC Research Article of the Year Award, and the SSPC Academic Collaboration of the Year Award. SM was previously awarded the UL President's Research Excellence and Impact Award (2022). SM has also secured competitive research funding from Research Ireland, the Alexander von Humboldt Foundation, the European Commission, and the Royal Society of Chemistry. With >110 peer-reviewed publications and >10,000 citations in materials chemistry, SM's research team, the *Mukherjee Group* (https://www.mukherjeegroup.ie/), develops porous adsorbent materials, including organic and metal-organic polymers to address the global grand challenges in chemical purification, air, and water treatment.