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CARES Visiting Scientist Seminar Series:

Mechanistic Insights into Nanoscale Separation and Catalytic Phenomena Using Multi-Scale Simulations and Machine Learning

Dr Ananth Govind Rajan; Department of Chemical Engineering,
Indian Institute of Science

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C4T Cambridge Centre for Carbon Reduction in Chemical Technology

Abstract: Catalytic carbon dioxide (CO2) conversion and membrane separations can enable energy efficient chemical industries. Our group combines quantum-mechanical density functional theory (DFT) calculations, molecular dynamics (MD), and kinetic Monte Carlo (KMC) simulations, with machine learning (ML), to understand the molecular underpinnings of separations and catalysis using nanomaterials. In this talk, I will present our recent work on understanding the atomic-level structure of nanopores in two-dimensional (2D) materials, which are important from the perspective of developing high-efficiency separation membranes. Specifically, I will discuss the combined use of DFT calculations, KMC simulations, and chemical graph theory to predict exact nanopore shapes in 2D graphene and hexagonal boron nitride (hBN) in excellent agreement with microscopy images. I will introduce the use of gradient-boosted ML strategies, coupled with structural features of nanopores, to predict the probabilities and formation times of arbitrary nanopore shapes in graphene. I will also outline the development of a novel string representation of nanopores in 2D materials, which enables the application of neural networks to develop structure-property relationships for nanoporous 2D materials. Finally, I will discuss our work on computational catalysis, wherein we unravel new mechanisms for electrochemical CO2 reduction to chemicals on pure/doped copper and 2D materials. I will also explain the development of ML models to predict activation (free) energies of elementary chemical reactions on catalyst surfaces using various physical features of adsorbate species and chemical transformations. Coupled with automated reaction enumeration strategies, the use of such ML models allows the exploration of complex reaction pathways involving thousands of elementary steps, and thus makes more realistic predictions of catalytic turnover frequencies for carbon dioxide reduction. Overall, the multi-scale simulations and ML algorithms presented in this talk will help understand and advance the use of 2D materials and single-atom alloys for separation and catalysis applications.

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