DEPARTMENT OF CHEMICAL ENGINEERING,
INDIAN INSTITUTE OF TECHNOLOGY KANPUR.

RESEARCH
SCHOLARS' DAY
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# Research Scholars' Day

ChE@IITK

April 10, 2025

2025

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*"Ignite Innovation, Engineer the Future!"*

# Message from Head

**Prof. Nitin Kaistha**
*Professor and Head,*
*Department of Chemical Engineering, IIT Kanpur.*

In our department, the research scholars are the ones driving the state-of-the-art research to address contemporary problems in the frontiers of chemical engineering (ChE). The systematic in-depth research conducted over postgraduation years under the able guidance of our faculty, enhances the students' research acumen and scholarly aptitude as they evolve, slowly but surely, from fledglings to seasoned scientists/researchers. To celebrate their work and also to provide a platform for showcasing the phenomenal research being carried out in the department, we organize the Research Scholars' Day (RSD) as a one day symposium consisting of a keynote lecture under the aegis of the CV Seshadri distinguished lecture series by a young ChE academician from within India, a general talk by a seasoned academician followed by oral talks by our senior research scholars and a poster session. On behalf of the department, I take this opportunity to invite you to 2025's ChE RSD edition on April 10th, which has certainly grown in quantity and hopefully in quality too.

This time around, we have Prof Jitendra Sangwai from IIT Madras presenting his work on subsurface chemical engineering and carbon capture and sequestration, Prof Deepak Kunzru familiarizing us with recent advances in ChE, 20 student oral talks in two parallel sessions and 28 poster presentations. The RSD talks and posters are representative of our major research verticals spanning complex fluids and soft matter; materials science; reaction engineering; energy and sustainability; theory, computations and machine learning and biosystems. It is our earnest hope that the 2025 RSD edition generates new perspectives and ideas while also enabling organic collaborations that propel our research to the next level.

Finally, it is worth highlighting that the RSD is entirely a student initiative organized for the ChE academic community. On behalf of the department, I take this opportunity to thank all the student volunteers as well as the supporting faculty and staff who have worked relentlessly behind-the-scenes to organize the event. We all Look forward to an invigorating and intellectually stimulating RSD on April 10th.

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# Research Scholars' Day 2025

## Department of Chemical Engineering, Indian Institute of Technology Kanpur.

## April 10, 2025

| Time | Event |
|---|---|
| 08:30 – 09:00 | Opening Ceremony (Venue: L17) |
| 09:00 – 09:50 | C.V. Seshadri Memorial Distinguished Lecture 2025 by **Prof. Jitendra Sangwai**, *"I am the Subsurface Reservoir"* (Venue: L17) |
| 09:50 – 10:40 | Research Scholars' Day 2025 Invited Talk by **Prof. Deepak Kunzru**, *"Recent Advances in Chemical Engineering"* (Venue: L17) |
| 10:40 – 11:00 | **Morning Tea** (Venue: L16 - L17 Foyer) |

| Time | Oral Talks Session 1 (Venue: L17) | Oral Talks Session 2 (Venue: L16) |
|---|---|---|
| 11:00 – 11:20 | *Influence of Diffusio-osmotic Flow on Colloidal Transport in Dead-End Pores* by **Jitendra Dhakar** | *Novel Algorithms for Efficient Exploration of Potential Energy Surfaces* by **Sandra Liz Simon** |
| 11:20 – 11:40 | *Speed-Accuracy Trade-Off in the Simulation of Realistic Arterial Blood Flow: Effects of Geometric Simplifications and Non-Newtonian Models* by **Rishi Kumar** | *Selective detection of riboflavin biomolecule over LIG-anchored iron nanoparticles using spectroelectrochemistry* by **Dhruv Chauhan** |
| 11:40 – 12:00 | *Clustering in Active Janus Colloids* by **Harishwar R** | *Predictive PI Averaging Level Control for Plantwide Applications* by **Aayush Gupta** |
| 12:00 – 12:20 | *Soliton in Liquid Crystals: Nanoparticles impact on solitons velocity, distance, and trajectory* by **Praveen Kumar Singh** | *Atomistic simulation of Type-I Mycobacterium tuberculosis Fatty Acid Synthase to unravel Acyl Carrier Protein shuttling mechanism at dehydratase* by **Manisha Sharma** |
| 12:20 – 12:40 | *Effect of anisotropy on the polymer diffusive instability in viscoelastic plane Couette flow* by **Shruti Pandey** | *A comparative assessment of 'standalone' PVDF membranes used in membrane distillation for hypersaline desalination* by **Joel Parayil Jacob** |
| 12:40 – 13:00 | *Electrified Sessile Droplets: Role of Bulk Charges, Surfactants and Substrate Elasticity* by **Shreyank Goel** | *Assessing the Synergies of Thermochemical Energy Storage with Concentrated Solar Power and Carbon Capture* by **Nitin Dhanenjey R** |
| 13:00 – 13:20 | *Hoop stress and polymer diffusive instabilities in viscoelastic Taylor-Couette flow* by **Pratyush Kumar Mohanty** | *An Efficient Method for Computing Ewald Summation with 2D Periodicity* by **Prateek Kumar Pandey** |
| 13:20 – 14:40 | **Lunch** (Venue: Outreach Lawn) | |
| 14:40 – 15:00 | *Fast and Accurate Numerical Methods for Evaluating Constitutive Models under Oscillatory Shear* by **Shivangi Mittal** | *Regenerable Fe-Ag-CNF Catalyst for Industrial Wastewater Treatment via Catalytic Wet Air Oxidation* by **Rahul Gupta** |
| 15:00 – 15:20 | *Sustainable Glycerol Carbonate Manufacturing: Process Synthesis, Design & Control* by **Prakhar Srivastava** | *Interval Hessian-based Optimization Algorithm* by **Ashutosh Sharma** |
| 15:20 – 15:40 | *Exploring integration of MOF- Hydrocarbons for sustainable adsorption-based cooling: An accelerated approach using Bayesian Optimization and Monte Carlo Simulations* by **S Muthu Krishnan** | — |
| 15:40 – 16:00 | **Evening Tea** (Venue: L16 - L17 Foyer) | |
| 16:00 – 17:30 | **Poster Presentations** (Venue: L19 - L20 Foyer) | |
| 17:30 – 18:00 | **Felicitation Ceremony and Vote of Thanks** (Venue: L17) | |

# C.V. Seshadri Memorial Distinguished Lecture 2025

## *I am the Subsurface Reservoir*

**Prof. Jitendra Sangwai**
Indian Institute of Technology Madras, Chennai.

10th April 2025, IIT Kanpur.

## Abstract

I am the subsurface reservoir, a hidden yet vital force in advancing sustainable energy futures and enhancing climate resilience. The modern world owes much of its progress to my role in supplying hydrocarbons, which have powered industries and societies for over a century. However, as the world transitions to cleaner energy resources, my role is evolving. While I will continue to support sustainable energy needs in the foreseeable future, I am being repurposed from a reservoir of fossil fuels into a critical asset for carbon capture and sequestration (CCS). My deep formations, both onshore and offshore, offer safe, long-term storage of carbon dioxide, preventing its release into the atmosphere. I also hold untapped potential, offering natural gas from hydrate reservoirs and possibly white hydrogen to meet energy demands while driving a sustainable future. Unlocking these possibilities requires a deeper, multidisciplinary understanding of my structure, processes, and long-term behavior to develop innovative technologies. Today, I stand at the intersection of energy security and climate accountability, bridging the past, present, and future of the global energy system.

This talk will focus on the sustainable production of hydrocarbons, as well as subsurface hydrogen storage and production, while integrating CCS strategies to build a sustainable energy future.

## Brief Bio of Speaker

Dr. Jitendra Sangwai is a Professor at the Department of Chemical Engineering, IIT Madras. He earned his Ph.D. with Professor Santosh K Gupta at IIT Kanpur and M.Tech. with Prof. Sirshendu De at IIT Kharagpur. Before academia, he worked briefly with Schlumberger. His research interests are in carbon capture and sequestration and upstream oil and gas engineering. He has published 180 international journal papers, holds 25 Indian and 18 international patents, and has mentored 25 Ph.D. graduates, many of whom are faculty at IITs, RGIPT, and in industry.

Government of India recognized him with the National Geoscience Award, and three National Awards for Technology Innovation. Society of Petroleum Engineers (SPE) bestowed him with the Distinguished Faculty Achievement Award. At IIT Madras, he is the first to win all the three major faculty awards, viz., Young Faculty Recognition Award, Institute Research and Development Awards (both at Early- and Mid-Career level) for excellence in teaching and research.

He is recognized as a Top 3% Highly Cited ACS Authors from India, ACS's Most Cited Author of Energy & Fuels, Top 1% Highly Cited Author of the I&ECR, and featured as an ”Emerging Investigator” on the cover page of Journal of Chemical and Engineering Data. He is an Associate Editor of Energy & Fuels and a Fellow of the Indian National Academy of Engineering.

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# Research Scholars' Day Invited Talk 2025

## *Recent Advances in Chemical Engineering*

**Prof. Deepak Kunzru**
School of Engineering and Applied Science, Ahmedabad University, Ahmedabad.

10th April 2025, IIT Kanpur.

## Abstract

Chemical engineering has witnessed significant advancements in recent years, driven by sustainability, digitalization, and material innovation. One of the most notable developments is the rise of green chemistry and sustainable processes. Researchers are focusing on bio-based feedstocks, carbon capture and utilization and energy-efficient chemical reactions to reduce industrial emissions. Electrochemical and photocatalytic methods for converting carbon dioxide into fuels and valuable chemicals have gained traction. Advances in materials and nanotechnology are revolutionizing catalysis, separation processes, and energy storage. In the biomedical field, nanoparticles are being engineered for targeted drug delivery, and development of more affordable diagnostic.

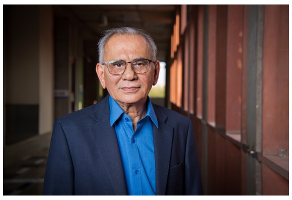
Process intensification is transforming traditional chemical engineering methods. Microreactors, with their high surface-area-to-volume ratios, are enabling continuous manufacturing processes that are both efficient and safer. Advancements in membrane technologies are optimizing separation processes, reducing energy consumption and operational costs. There have been significant advances in biotechnology and biochemical engineering, including the development of biorefineries , biodegradable plastics and engineered microbes for various applications. The applications of AI in chemical engineering is ushering in a new era of innovation.

This talk will highlight some of the recent innovations in chemical engineering that are helping to address global challenges such as climate change, energy security, and resource scarcity.

## Brief Bio of Speaker

Prof. Deepak Kunzru is Dean, Graduate School Research and Distinguished Professor, School of Engineering and Applied Science at Ahmedabad University. He superannuated as Professor of Chemical Engineering from IIT Kanpur in 2016. He obtained his B.Tech. from IIT Kanpur in 1968 and Ph.D. from the University of Pittsburgh in 1972. He was a Visiting Professor at MIT (2009) and held the Chevron Chair Professorship at IITK.

His research spans microstructured reactors, chemical reaction engineering, petroleum processing, and $CO_2$ utilization. He has led 20 research projects, published over 110 papers, and edited one book. At IIT Kanpur, he served as Head of the Department, Dean (R&D), and Dean (Resource Planning). He has been an expert in several national committees, including DST/SERB and HPCL Corporate R&D.



Prof. Kunzru is a Fellow of INAE (2002) and NASI (2009). His accolades include the Herdillia Award (IIChE, 1992), Kuloor Memorial Award (1999, 2015), and the IIT Kanpur Institute Fellow Award (2022). He has delivered distinguished lectures at leading institutions and contributed significantly to chemical engineering education and research.

# Abstracts for Oral Talk Session-1

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# Influence of Diffusio-osmotic Flow on Colloidal Transport in Dead-End Pores

Jitendra Dhakar, Kushagra Tiwari, and Akash Choudhary
*Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*

## Abstract

Electrolytic diffusiophoresis and diffusioosmosis refer to the directional migration of colloids and fluid due to interfacial forces that develop in response to local electrolytic gradients ($\beta$). This physicochemical transport provides an efficient alternative in numerous microscale applications where advection-induced transport is infeasible. Phoretic withdrawal and injection in dead-end pores can be controlled by osmotic wall slip; however, the extent to which this wall slip influences spatiotemporal transport patterns for different gradient orientations is not thoroughly explored. This study numerically analyzed the influence of diffusioosmotic wall slip on colloidal withdrawal and injection dispersion for different solute gradient orientations (solute-out, i.e., solute emptying pore and solute-in, i.e., solute saturating pore). We find that the osmosis-induced mixing can enhance withdrawal (solute-out/-in mode) and injection (solute-in mode) effectiveness, whereas it counterintuitively inhibits injection effectiveness in solute-out mode. These insights improve the understanding of colloidal dispersion driven by osmotic flow in different phoretic transport modes and contribute to the systematic design and optimization of electrolytic gradient configurations.

**Keywords:** Diffusioosmosis, Diffusiophoresis, Electrolytes, Dead-end pore.

# Speed-Accuracy Trade-Off in the Simulation of Realistic Arterial Blood Flow: Effects of Geometric Simplifications and Non-Newtonian Models

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[1]*Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*
[2]*Department of Mechanical Engineering, Indian Institute of Technology Kanpur, India*

## Abstract

Recent developments in computational fluid dynamics have enabled studies of blood flow in realistic arterial geometries. Thus, it is possible to compute flow distribution in three dimensions for pulsatile flow in branches and bifurcations with bulges and constrictions. When the geometry is made realistic, undulations and perturbations of the artery wall need refinement in mesh size, thereby increasing computational cost. Secondly, for accurate representation of a complex fluid such as blood, non-Newtonian blood rheology models need to be used, further increasing complexity. In the present study, we explore the consequences of simplifying geometry in the context of a variety of blood viscosity models. The original artery model is obtained from CT scans and progressively simpler geometries are generated by a process of smoothening. In these equivalent geometries, we study blood flow aspects using both Newtonian and non-Newtonian rheology. The goal is to examine the accuracy-speed tradeoff for patient-specific artery models and the extent to which the flow details are compromised. We solve the incompressible continuity and momentum equations with blood viscosity mod- els incorporating realistic pulsatile boundary conditions. A finite volume method-based solver in OpenFOAM-10 is adopted on an unstructured mesh. Blood rheology models studied vary from the Newtonian, Carreau-Yasuda, to the recently formulated Apostolidis-Beris model, with and without the diffusive fluxes that represent particle migration. Results are presented for a descending aorta along with its simpler versions obtained by averaging diameter over short arterial segments. Three levels of equivalent geometry are studied. Level 1 is the original derived from DICOM images provided by a medical hospital. For Level 2, the entire artery is divided into slices along its length, with each slice represented as a smooth duct of constant diameter. Level 3 is a straight circular tube whose inlet and exit diameters are matched with the original. Inlet flow waveform is specified in terms of the peak flow rate and frequency; rest and exercise conditions are separately analyzed. The outcomes of simulation are shown in terms of vortical patterns and other hemodynamic parameters such as wall shear stress (WSS), time average wall shear stress (TAWSS), and oscillatory shear index (OSI) for each of the blood viscosity models. Differences in flow patterns among the three levels are minor while the reduction in CPU time is substantial. However, quite a few essential details are lost in Level 3 where undulations are smoothed out and is not recommended. Our study is a new attempt to simplify complex arterial networks so as to enable meaningful full body simulations in real time.

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# Clustering in Active Janus Colloids

Harishwar Raman[1], Karnika Singh[1], Akash Choudhary[1] and Rahul Mangal[1]
[1]*Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*

## Abstract

In this study, we experimentally investigate the dynamics of chemically active $SiO_2$-Pt Janus Colloid (JC) clusters in a dynamic clustering state, where clusters continuously form, break, or merge as their population increases. These size-monodisperse active JCs exhibit cluster dynamics strongly influenced by the orientations of individual particles within the cluster. Our findings reveal that the translational and rotational motions of a cluster can be effectively predicted by considering the individual particle orientations, offering a robust framework for understanding cluster behavior across varying sizes. We also demonstrate how the interactions between a pair of active JCs impacts cluster formation and consequently, the cluster movement. This work establishes a generalizable approach to predicting the motion dynamics of active JC clusters and underscores their potential for applications requiring precise control of morphology and movement.

# Soliton in Liquid Crystals: Nanoparticles impact on solitons velocity, distance, and trajectory

Praveen Kumar Singh, Soumik Das

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## Abstract

Solitons are wave packets that maintain their shape while propagating at a constant speed over long distances. A nonlinear feedback mechanism that counteracts dispersion during their travel is responsible for this shape retention. Solitons have been thought to be involved in biological processes like signal propagation along neurons and have been seen in a variety of natural circumstances, including the movement of water waves along shallow canals.

Recent studies suggest that solitons can be used for long-distance signal transmission Das et al., 2022 and Tang et al., 2024. In this work, we used the liquid crystal 4-butyl-4-heptyl-bicyclohexyl-4-carbonitrile (CCN-47) to create a nanocomposite of two distinct nanoparticles. In CCN-47, titanium oxide ($TiO_2$) and barium titanate ($BaTiO_3$) nanoparticles were dispersed in three concentrations. Both nanoparticles have demonstrated an effect on the strength of the electric field where the solitons are present.

ImageJ software is used to calculate velocity, total distance, and trajectory. The obtained result indicates that, in the case of a $BaTiO_3$ dispersed system, the solitons' travel distance increases while their velocity decreases. Overall, the findings in the realm of soft matter nanoscience are quite intriguing.

## References

Das, Soumik et al. (2022). "Programming solitons in liquid crystals using surface chemistry". In: *Langmuir* 38.11, pp. 3575–3584.

Tang, Xingzhou et al. (2024). "Generation and propagation of flexoelectricity-induced solitons in nematic liquid crystals". In: *ACS nano* 18.16, pp. 10768–10775.

# Effect of anisotropy on the polymer diffusive instability in viscoelastic plane Couette flow

Shruti Pandey[1] and V. Shankar[1]

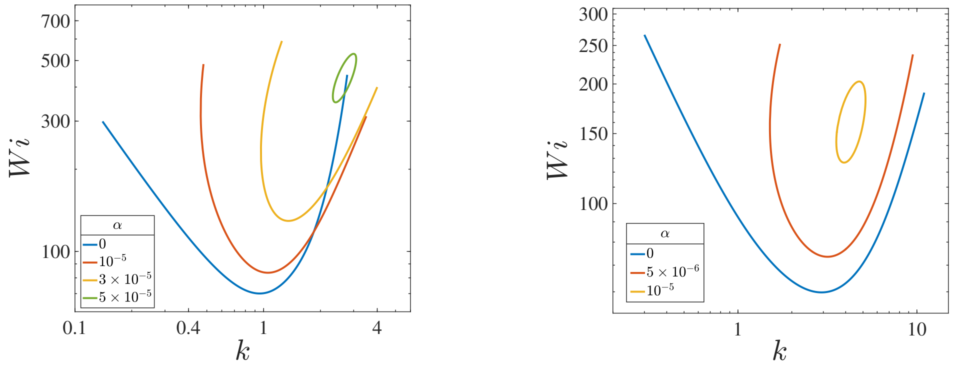
[1] *Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*

## Abstract

The present work focusses on the linear stability analysis of inertialess viscoelastic plane Couette flow using the non-linear Giesekus model, which not only accounts for an anisotropic drag coefficient, but also predicts shear thinning of viscosity. The Giesekus constitutive relation augmented by a stress diffusion term is given by:

$$\boldsymbol{\tau} + Wi\left(\frac{\partial \boldsymbol{\tau}}{\partial t} + \boldsymbol{v}.\boldsymbol{\nabla}\boldsymbol{\tau} - \boldsymbol{\nabla}\boldsymbol{v}^T.\boldsymbol{\tau} - \boldsymbol{\tau}.\boldsymbol{\nabla}\boldsymbol{v}\right) + \frac{\alpha Wi}{(1-\beta)}(\boldsymbol{\tau}\cdot\boldsymbol{\tau}) = (1-\beta)(\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^T) + \mathcal{D}\nabla^2\boldsymbol{\tau}. \tag{1}$$

Plane Couette flow has been found to be linearly unstable if polymer stress diffusion is included in the Oldroyd-B fluid (Chokshi and Kumaran, 2009). The unstable mode has been termed as the polymer diffusive instability (abbreviated PDI hereafter) (Beneitez, Page, and Kerswell, 2023).The conventional (non-diffusive) Giesekus model predicts plane Couette flow to be linearly stable (Grillet et al., 2002). A similar analysis is carried out for the homogeneous diffusive Giesekus model using two different boundary conditions: no-flux and no-diffusion.



(a) No-flux boundary condition (b) No-diffusion boundary condition

Figure 1: Neutral curves in the $Wi$-$k$ plane for the diffusive Giesekus model at different $\alpha$ for $Re = 0$, $\mathcal{D} = 0.1$ and $\beta = 0.92$.

Our numerical results reveal that the PDI stabilises rapidly as anisotropic coefficient ($\alpha$) increases, resulting in the shrinking of the neutral curves in the $Wi$–$k$ plane, for both boundary conditions, as shown in Fig.1. For solvent to solution viscosity ratio $\beta = 0.92$, the system stabilises rapidly at smaller values of $\alpha$ ($O(10^{-5})$). For concentrated solutions, the system requires

higher anisotropic coefficient ($O(10^{-3})$) to stabilize itself at very low $Wi$. The stabilization of the polymer diffusive instability is clearly due to the anisotropic effects irrespective of the shear thinning nature of the Giesekus model. The PDI is found to be extremely sensitive to the boundary conditions.

## References

Beneitez, Miguel, Jacob Page, and Rich Kerswell (Oct. 2023). “Polymer diffusive instability leading to elastic turbulence in plane Couette flow”. In: *Phys. Rev. Fluids* 8 (10), p. L101901. DOI: `10.1103/PhysRevFluids.8.L101901`.

Chokshi, P. and V. Kumaran (2009). “Stability of the plane shear flow of dilute polymeric solutions”. In: *Phys. Fluids* 21, p. 014109. DOI: `10.1063/1.3063893`.

Grillet, A.M. et al. (2002). “Stability analysis of constitutive equations for polymer melts in viscometric flows”. In: *Journal of Non-Newtonian Fluid Mechanics* 103 (2-3), pp. 221–250. DOI: `https://doi.org/10.1016/S0377-0257(02)00005-8`.

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# Electrified Sessile Droplets: Role of Bulk Charges, Surfactants and Substrate Elasticity

Shreyank Goel[1], and Dipin S. Pillai[1]
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## Abstract

Miniaturization is crucial in today's world, with microfluidics enabling the integration of multiple processes on a single chip. In droplet-based microfluidics, applying an external electric field allows precise control over droplet mixing, transport, and manipulation. The behavior of sessile droplets is primarily governed by the triple-phase contact line (TPCL), which we analyze using thin-film modeling. This study has implications for low-Reynolds-number mixing, electrovariable optics, droplet actuation, and bioassays. We investigate three key aspects of electrohydrodynamic phenomena in digital microfluidics: (a) the influence of bulk charges on electrowetting, (b) electrowetting of surfactant-laden sessile droplets, and (c) the statics and dynamics of electrowetting and dewetting on soft dielectrics (EWSD/EDSD). The electrowetting behavior of charge-carrying electrolytic and surfactant-laden droplets is relevant to applications like point-of-care diagnostics. Biomedical assays often involve droplets containing charged molecules, such as dissolved ions, proteins, and DNA, along with surfactants like those found in respiratory droplets. In the first part, we develop a reduced-order electrokinetic model for electrowetting of charge-carrying droplets in a parallel-plate electrode configuration. We demonstrate that electrolytic droplets can deform more than perfect conductors or dielectrics, depending on the Debye length. In second part, we present a theoretical model for electrowetting of surfactant-laden droplets, showing that surfactants suppress electrohydrodynamic flow due to Marangoni stress. The response to an AC field results in reduced oscillation amplitude while maintaining the same mean deformation as under DC forcing . Finally, we have studied the role of elasticity on electro(de)wetting. Our findings reveal that increased substrate softness and viscoelastic dissipation slow down droplet spreading, aligning with previous experimental observations.

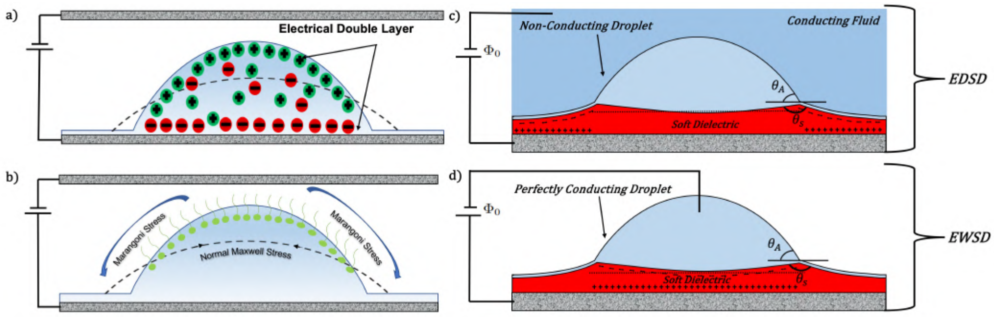


Figure 1: Schematic of **(a)** charged and **(b)** surfactant laden droplet under parallel plate electrode configuration. Schematic of **(c)** electrodewetting and **(d)** electrowetting over soft dielectric configuration.

# Hoop stress and polymer diffusive instabilities in viscoelastic Taylor-Couette flow

Pratyush Kumar Mohanty[2], P.S.D Surya Phani Tej[1] and V. Shankar[1]

[1] *Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*

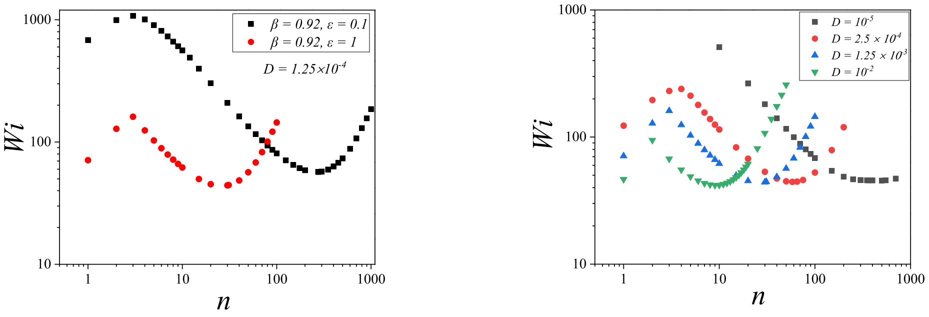
[2] *Department of Chemical Engineering, National Institute of Technology Rourkela, India*

## Abstract

Viscoelastic fluids are known to exhibit 'purely elastic' linear instabilities in curvilinear geometries like the Taylor-Couette or Dean flow configurations. These instabilities, driven by hoop stresses, are even present in the absence of inertia. The present study accurately predicts the purely elastic HSM instability in the finite gap limits. Recent direct numerical simulations (DNS) of two-dimensional Taylor–Couette flow reveal the presence of a linear instability that does not correspond to the well-known HSM, which is inherently absent in two-dimensional configurations. To investigate the origin of this instability, we introduce polymeric diffusion, drawing parallels with the role of artificial viscosity in numerical simulations. The Oldroyd-B constitutive relation along a stress diffusion term is given by:

$$\boldsymbol{\tau} + Wi\left(\frac{\partial \boldsymbol{\tau}}{\partial t} + \boldsymbol{v}.\boldsymbol{\nabla}\boldsymbol{\tau} - \boldsymbol{\nabla}\boldsymbol{v}^T.\boldsymbol{\tau} - \boldsymbol{\tau}.\boldsymbol{\nabla}\boldsymbol{v}\right) = (1-\beta)(\boldsymbol{\nabla}\boldsymbol{v} + \boldsymbol{\nabla}\boldsymbol{v}^T) + \mathcal{D}\nabla^2\boldsymbol{\tau}. \tag{1}$$

The polymeric diffusive instability (PDI) has been predicted in plane Couette flow (Beneitez, Page, and Kerswell, 2023). We also obtained the PDI for the curvilinear Taylor-Couette configuration. We have carried out our analysis using the no-diffusion boundary condition for the polymeric stress diffusion.



(a) Different gap widths ($\epsilon$) at $\mathcal{D} = 0.00125$

(b) Different diffusivities ($\mathcal{D}$) at $\epsilon = 1$

Figure 1: Neutral curves in the *Wi*-*n* plane for the diffusive Oldroyd-B model for $Re = 0$ and $\beta = 0.92$.

Our numerical results reveal regardless of the polymer stress diffusivity ($\mathcal{D}$) value, there is no significant change in $Wi_c$; only the value of the azimuthal wavenumber $n$ at which Wi becomes critical changes. The HSM is stabilized as diffusivity is increased. Till now, PDI has been reported only in 2D and was therefore considered a purely 2D instability. However, we demonstrate that PDI persists significantly in 3D limit as well. As $\alpha$ increases gradually, it tends to stabilize the PDI mode. However, the stabilization is not very prominent, as PDI persists even at $\alpha$ as high as 40.

# References

Beneitez, Miguel, Jacob Page, and Rich Kerswell (Oct. 2023). "Polymer diffusive instability leading to elastic turbulence in plane Couette flow". In: *Phys. Rev. Fluids* 8 (10), p. L101901. DOI: `10.1103/PhysRevFluids.8.L101901`.

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# Fast and Accurate Numerical Methods for evaluating Constitutive Models under Oscillatory Shear

Shivangi Mittal[1], Yogesh M. Joshi[1], and Sachin Shanbhag[2]

[1]*Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*
[2]*Department of Scientific Computing, Florida State University, Tallahassee, Florida, USA*

## Abstract

Large amplitude oscillatory shear (LAOS) flow is a promising rheological protocol for understanding the nonlinear viscoelastic properties of complex fluids. Experimental LAOS data are especially useful when they can be associated with constitutive theories that describe the underlying physics. Constitutive models (CMs) are systems of integral or differential equations in stresses and strain, which may or may not possess analytical closed-form solutions when subjected to a LAOStrain input. In this work, we present an alternate approach to solve nonlinear differential CMs for LAOS flows, as opposed to conventionally used numerical time-stepping algorithms. This method, called Harmonic Balance (HB), belongs to the class of Fourier-Galerkin weighted residual methods. HB outperforms conventional methods both in terms of accuracy and speed, often by several orders of magnitude.

We first briefly discuss the formulation of equations and implementation of HB for different CMs. The system of differential equations in the time domain is transformed into an optimization problem in the frequency domain, with Fourier coefficients of stress (and not stress itself) becoming the unknown variable. As expected, the HB solution has superior convergence and accuracy compared to conventional numerical time-stepping algorithms and even analytical solutions. Subsequently, we discuss a unique mechanism to generalize HB to any nonlinear differential CM using an alternating frequency time scheme. Finally, we also touch upon an analogous, more efficient Fourier-based numerical approach for integral constitutive CMs.

These spectral methods unleashes new domains for theoretical analysis by making LAOS computations cheaper, such as model calibration and model selection for experimental data, thermodynamic stability analysis, and mathematical instabilities in CMs.

# Sustainable Glycerol Carbonate Manufacturing: Process Synthesis, Design & Control

Prakhar Srivastava[1] and Nitin Kaistha[1]

[1] *Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*

## Abstract

A proposed economic steady-state process design is developed for valorizing glycerol, a co-product of biodiesel manufacturing, to glycerol carbonate (GC) via transesterification with dimethyl carbonate (DMC). Methanol is a co-product of the reaction. The process flowsheet is synthesized using residue curve maps and consists of a pressurized reactive distillation (RD) column followed by three low-pressure simple distillation columns. The sensitivity of the MeOH-DMC azeotrope to pressure is exploited to recover pure MeOH co-product and recycle the unreacted DMC. Comparison with recently published RD pervaporation (RDPV)(Sun et al., 2022) and RD extractive distillation (RDED)(Yu, 2020) process designs shows their cost objective to be respectively 47% and 20% higher than the proposed design. The energy consumption per kmol GC product is also higher by 12% and 26% respectively. Rigorous dynamic simulations show that the developed process design has good controllability with a traditional decentralized plantwide control system effectively handling the principal disturbances with tight product quality control.

## References

Sun, Dayu et al. (2022). "Process Design, Economic Optimization, and Environmental Assessment for the Production of Glycerol Carbonate via Reactive Distillation Combined with Pervaporation". In: *Industrial & Engineering Chemistry Research* 61.44, pp. 16552–16564.

Yu, Bor-Yih (2020). "Development of two plant-wide glycerol carbonate production processes: Design, optimization and environmental analysis". In: *Journal of the Taiwan Institute of Chemical Engineers* 117, pp. 19–25.

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# Exploring integration of MOF- Hydrocarbons for sustainable adsorption based cooling: An accelerated approach using Bayesian Optimization and Monte Carlo Simulations

S. Muthu Krishnan[1] and Jayant K Singh[1]

[1]*Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*

## Abstract

Global warming has made summers extremely miserable, especially for Tier I and II cities, making daily life impossible without ACs. The vapor compression cycles (VCCs) employed in ACs utilize a refrigerant that is predominantly hydrofluorocarbons with high global warming potential (GWP) and a compressor that operates on electricity. This pushes for extreme constraints on the energy grid in summers, necessitating the need to look beyond VCCs for cooling. Adsorption-based cooling systems (ARCs) offer a promising alternative (Krishnan and Singh, 2025; Krishnan, Sharma, and Singh, 2024), by replacing the compressor with an adsorbent bed, which regenerates using low-grade heat sources like waste heat and solar energy, thus eliminating the dependence on electricity. The efficiency of the ARC primarily relies on the adsorbent bed and refrigerant used.

Metal-Organic Frameworks (MOFs) have proven to be superior adsorbents than their predecessors with their high sorption capacity, surface area, and customizable structural and chemical properties, opening up the possibility of their integration in ARCs. Application of ARCs with MOFs has been explored in literature with refrigerants like ethanol, methanol, and water and has been shown to improve the efficiency of the cycle exceptionally than its predecessors, but their hypobaric vapor pressures make the practical application of the cycle difficult (Krishnan, Sharma, and Singh, 2024). Integration of MOFs in combination with the green hyperbaric refrigerants propane and isobutane will improve the efficiency without compromising the practicality of the cycle.

To this end, we performed Bayesian optimization (Daoo and Singh, 2024) based 3-level screening on the CoRE MOF Database to find the optimal COP that can be obtained from this cycle for MOF integrations with propane and isobutane refrigerants. We obtained a maximum COP of 0.725 and 0.786 for MOF-propane (Krishnan, Sharma, and Singh, 2024) and MOF-isobutane (Krishnan and Singh, 2025) integrations, respectively. This study revealed that for improved efficiency, the MOF should possess a high surface area, accessible volume, and void fraction, thus leading to a stepwise adsorption isotherm. Further, we improved the efficiency of this cycle by increasing the temperatures at which the regeneration of the adsorbent was performed, which leads to higher working capacity.

Further, given that the cascading of the adsorbents can improve the efficiency of this cycle, we performed active learning-based screening to find the optimal COP for various combinations of MOFs in cascaded fashion for propane and isobutane refrigerants. We obtained a maximum

COP of 1.67 and 1 for propane and isobutane refrigerants, respectively, which is a significant improvement from our previous analysis. This improvement in efficiency calls for the practical validation of the cycle. Moreover, we performed structure property relationships analysis to study their influence on the COP of this cycle; this revealed a similar analysis as in the previous study. But an interesting observation was that the influence of the structural properties on the COP of the cycle was more profound at high pressure than at low pressures.

My talk will explore the integration of MOFs as superior adsorbents combined with low-GWP refrigerants. I'll discuss finding the best adsorbent for this cycle through Bayesian optimization-based sampling of the dataset and the impact of MOF structural properties on the adsorption isotherms and its effect on the efficiency of the ARC. Moreover, my talk will also cover the adsorption isotherms observed in this cycle for different operating conditions and how this can be adjusted to improve the efficiency of this cycle. I'm hoping my talk will be of interest to several researchers working on MOF applications for adsorption cooling, $CO_2$ capture, and $H_2$ adsorption.

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# Abstracts for Oral Talk Session-2

RSD2025 ChE@IITK

# Novel Algorithms for Efficient Exploration of Potential Energy Surfaces

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# Abstract

## 1.1 Introduction

Efficient exploration of the potential energy surface (PES) and identification of minimum energy paths (MEPs) and transition states (TSs) are essential for understanding chemical reaction mechanisms. The Nudged Elastic Band (NEB) method is a popular approach for MEP discovery [1]. However, its dependence on quantum mechanical (QM) calculations for energy and force evaluations makes it computationally demanding, particularly for systems with hundreds to thousands of atoms. For instance, methane decomposition over molten catalysts involves approximately 1000 atoms and 4000 electrons. A typical NEB calculation for such a system requires approximately 5000 steps (or 40000 quantum chemical evaluations) to converge. A calculation on HPC with 4 nodes and 48 cores each (2.9 GHz, 4 GB per core), only 15 steps can be completed per hour, requiring at least 15 days to converge. To tackle this substantial computational expense, we have developed two new algorithms: AARE and AL-NEB, that can efficiently explore PES and accelerate the study of reaction mechanisms.

## 1.2 Methodology

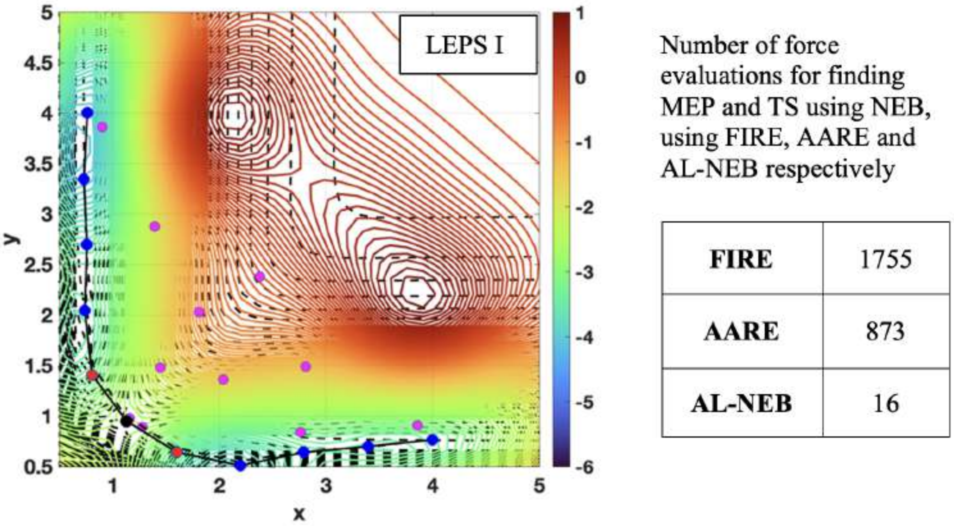
### 1.2.1 Development of optimization algorithm

An effective way to reduce computational cost is by employing a more efficient algorithm for optimizing NEB forces. Force-based optimizers, such as the Fast Inertial Relaxation Engine (FIRE), are commonly used for this purpose [2]. However, FIRE has notable limitations, including dependence on an empirical mixing parameter and issues with convergence speed due to braking during uphill motion, short latency time, and overshooting. To overcome these challenges, we developed the Adaptively Accelerated Relaxation Engine (AARE), which enhances molecular dynamics trajectories through an adaptive acceleration scheme that utilizes local information and a conjugate gradient-like direction.

### 1.2.2 Development of an active learning algorithm for finding transition state

Another effective approach involves leveraging the machine learning technique, Gaussian Process Regression (GPR), to construct a model PES for chemical reactions [3]. Building on this, we have developed a novel Active Learning NEB (AL-NEB) algorithm, which employs an exploration-exploitation-renunciation strategy to identify transition states on the PES efficiently. The algorithm learns the true PES from a limited, strategically selected set of data points, with their energies and forces computed using Gaussian16 software [4]. By utilizing GPR-predicted energies and forces instead of computationally expensive quantum mechanical calculations during NEB optimization, AL-NEB reduces the computational cost by an order of magnitude, making it a highly efficient tool for reaction mechanism studies.

## 1.3 Findings



Number of force evaluations for finding MEP and TS using NEB, using FIRE, AARE and AL-NEB respectively

| | |
|---|---|
| **FIRE** | 1755 |
| **AARE** | 873 |
| **AL-NEB** | 16 |

Figure 1: MEP and transition state on the GPR-predicted surface for LEPS-I potential AL-NEB. Black contours represent the true PES, red dots are training points, and the blue dotted line is the final MEP with the black dot as the transition state. The table compares the computational costs of different algorithms.

- **Efficiency of AARE:** AARE reduces QM evaluations by over 50%, consistently outperforming the FIRE method on various PES and reaction systems.
- **Adaptive Nature of AARE:** AARE's adaptive acceleration and direction selection ensure gradual convergence, minimizing overshooting and crawling issues seen in FIRE.
- **Effectiveness of AL-NEB:** AL-NEB constructs an accurate model PES, enabling NEB calculations using predicted energies and forces. This reduces the need for QM evaluations by an order of magnitude, significantly improving computational efficiency.

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# Selective detection of riboflavin biomolecule over LIG-anchored iron nanoparticles using spectroelectrochemistry

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## Abstract

Developing efficient biomolecule sensors for quick and accurate analysis using biocompatible and sustainable materials is necessary in the current age. In this study, Riboflavin (RF) is detected via in situ spectroelectrochemistry (SEC) technique, utilising laser-induced graphene (LIG)-anchored iron nanoparticles (Fe NPs) modified fluorine tin oxide (FTO) glass electrode. The electrode fabrication involves a simple yet efficient process where a Fe-dispersed phenol-formaldehyde copolymeric film is converted to Fe-LIG in a single step using laser ablation. The SEC technique combines cyclic voltammetry with UV-Vis spectrophotometry to measure RF based on the 400 nm absorbance peak of its electro-reduced species. The Fe-LIG modification improves the sensitivity and charge transfer resistance by increasing its electrochemical surface area nearly threefold. The sensor demonstrates a wide linear detection range for RF concentrations, spanning from 0.05 to 40 µg/ml, with a low detection limit of 0.048 µg/ml. The sensor was tested in artificial and real urine samples, successfully replicating real-world sample analysis conditions. Moreover, the SEC sensor was tested in RF solutions containing various potential interferents. The results showed unaltered absorbance peak intensities for RF, suggesting robustness and reliability of SEC sensor, unlike standalone electrochemical or UV-Vis spectrophotometry techniques, which often suffer from peak convolution, distortion, or intensity alteration due to interfering substances during biomolecule sensing. The findings of this study provide broader prospective applications of inexpensive metal-LIG composite-based electrodes in conjunction with SEC techniques for interference-free detection of critical biomolecules.

# Predictive PI Averaging Level Control for Plantwide Applications

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## Abstract

This work develops a novel predictive Proportional-Integral (PI) Averaging Level Control (ALC) algorithm designed to fully utilize the available liquid surge capacity in surge tanks for flow transient smoothing while ensuring that the high and low alarm limits are not breached. The proposed algorithm incorporates a tunable parameter to mitigate flow overshoot in interconnected plantwide systems with material recycle. The performance of the algorithm is compared with existing popular ALC algorithms for a tanks-in-series with recycle process as well as a realistic dimethyl ether (DME) process and is found to be competitive with respect to manipulated flow variability mitigation for small to moderate disturbances. The algorithms also robustly handles extreme flow disturbances without level alarm violation. The significant flow variability mitigation with consequently lower back-offs from optimally active constraint limits results in up to 8.25% reduction in energy consumption and 4% higher maximum throughput compared to the conventional norm of using P-only ALC in plantwide systems for the DME process. The quantitative results highlight the significant potential of the proposed ALC algorithm towards efficient and sustainable process operation.

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# Atomistic simulation of Type-I Mycobacterium tuberculosis Fatty Acid Synthase to unravel Acyl Carrier Protein shuttling mechanism at dehydratase

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## Abstract

*Mycobacterium tuberculosis* (Mtb) fatty acid synthase type I (FAS-I) is an essential protein complex and a potential drug target. This complex consists of homo-hexameric chains with 7 domains per chain that catalyze the synthesis of fatty acid, which is a significant component of the cell wall of Mycobacteria. Of these domains, acyl carrier protein (ACP) is involved in shuttling a growing fatty acid across the 6-remaining domains in an iterative and sequential manner.

Incomplete structural details of Mtb FAS-I at near-atomic resolution have limited our understanding of the shuttling mechanism of its mobile acyl carrier protein (ACP). ACP shuttling mechanism is conserved across species like fungal. Gaining insights from this evolutionary trend, we have performed an atomistic molecular dynamics simulation of Mtb FAS-I with a homology-modelled structure of ACP stalled at low occupancy step: dehydratase (DH) and identified key residues mediating ACP anchoring near DH. The observed distance between ACP and DH catalytic residues agrees with that reported for fungal FAS-I. Further, the conformation of the peripheral linker is found to be crucial in stabilising ACP near DH.

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# A comparative assessment of 'standalone' PVDF membranes used in membrane distillation for hypersaline desalination

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## Abstract

Membrane Distillation (MD) can treat hypersaline feed or reverse osmosis reject and further improve freshwater recovery rate and reduce the amount of liquid discharge. However, inorganic scaling on membrane surfaces is a concern when treating hypersaline feed. Chemical modification using perfluoroalkyl silanes is a popular route to mitigate inorganic scaling on membrane surface for membrane distillation (MD). In this paper, we test for PVDF membranes with no chemical modification prepared via different non-solvent induced phase inversion routes for their performance in high propensity scaling conditions. Results reveal that the easiest among the three phase inversion techniques show excellent potential for delaying gypsum scaling. It is found that low pore size and a smooth membranes surface is advantageous in delaying scaling and this is confirmed via SEM, EDS and 3D AFM images. Cyclic runs using supersaturated (28mM) gypsum over a total period of 30 hours and treatment of real RO reject for 50 hours further confirm the potential of the best performing PVDF membrane. Since non-solvent induced phase separation is widely adopted as an industry standard for fabrication of polymeric membranes, the results in this work point towards an easily adaptable large scale membrane manufacturing of MD membranes for hypersaline feed

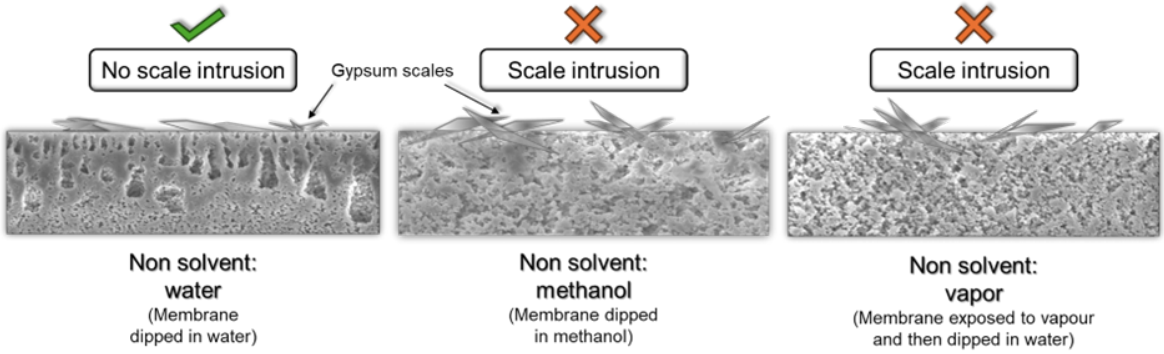

Figure 1: Different membranes and their response to hypersaline environment

# Assessing the Synergies of Thermochemical Energy Storage with Concentrated Solar Power and Carbon Capture

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## Abstract

As greenhouse gas emissions continue to increase worldwide, the growing energy demand must be met using low-carbon technologies. Two classes of technology that can mitigate $CO_2$ emissions are carbon capture and storage (CCS) and renewable energy generation. These two technologies have been primarily developed independently. However, their hybridization can offer complementary benefits and lower the costs of greenhouse gas abatement.

Concentrated solar power (CSP) with thermal energy storage (TES) is a promising strategy to deliver cost-effective, reliable, and dispatchable renewable power. Among various TES technologies, thermochemical energy storage (TCES) is especially appealing for the next generation CSP plants because of their high energy density and ability to deliver heat at a high temperature (>1000 °C). A recent material screening study (Bajaj, Peng, and Maravelias, 2024) concluded that due to the low energy density of TCES materials, even the most economically favorable reaction system leads to more than 50% higher LCOE than the monthly average electricity retail price.

Accordingly, we propose a novel carbon-neutral process (referred to as CSP-TCES-OFC) that integrates CSP and energy-dense fossil-fuel power plant with a redox-based TCES system. The CSP-TCES-OFC process operates as follows. During the day, the heliostats focus sunlight onto the receiver, where photons are absorbed, and heat transfer fluid (HTF) is heated. The flow of HTF is split such that one fraction drives the forward endothermic reaction ($M_xO_z \leftrightarrow M_xO_y + \frac{z-y}{2}O_2$), and the other heats the working fluid. The oxygen released due to the forward endothermic reaction is stored and used for fuel combustion during the night. The exhaust from fuel combustion mainly contains $CO_2$ and $H_2O$, which are cooled and separated using a flash column. The $CO_2$ stream is then compressed and stored underground. The reverse exothermic reaction to oxidize the reduced metal oxide occurs in the presence of air. Thus, during the night operation, energy is obtained by reversible exothermic reaction and combusting fuel.

We optimize the process' economic performance considering variability in solar irradiance by developing a two-stage stochastic programming model to obtain the optimal design, operating conditions, and system performance of the CSP-TCES-OFC plant. We illustrate that compared to the CSP-TCES process employing the $Mn_2O_3/Mn_3O_4$ TCES system, the proposed hybrid process has a 25% lower levelized cost of electricity (LCOE) for an 80% capacity factor. We also compare the economic performance of our process with another hybrid configuration containing CSP-TCES, boiler for fuel combustion, and air separation unit (ASU) to produce $O_2$, which is then used to combust fuel. We conclude that the LCOE of the proposed process is 11.5% lower than the LCOE of the process with an ASU.

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# An Efficient Method for Computing Ewald Summation with 2D Periodicity

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## Abstract

Accurate computation of long-range coulombic interactions is essential in molecular simulations, as they dominate other interactions, such as van der Waals. However, calculating these interactions can be computationally expensive, particularly for large-scale systems. Large-scale systems are typically modelled as a small simulation cell that is periodically repeated in all three dimensions. The traditional Ewald summation[1, 3] addresses the challenge of computing Coulombic interaction with complete 3D periodicity. It splits the Coulomb potential into two parts: a short-range component handled in real space and a long-range component in reciprocal space using Fourier transforms. The short-range part rapidly converges, while the long-range part uses Fast Fourier Transform (FFT) and interpolation techniques, which scales as $\mathrm{O}(N \log N)$ time complexity, where $N$ is the number of charged ions.

The Ewald method becomes more challenging for systems with reduced periodicity, such as 2D slab geometries. These systems are periodic in two dimensions and finite in the third, which disturbs the overall symmetry essential for fast computation of Ewald summation. Traditional or even modern approaches struggle with computational efficiency and accuracy for slab geometries. These methods often require complex corrections or approximations that render the simulations slower than 3D Ewald summation.

In this work, we propose a method of computing an exact 2D Ewald summation, which is more efficient than the 3D Ewald summation. Our approach utilizes a modified screening function for the reciprocal space summation within the Particle-Mesh Ewald (PME) method. Using FFT for reciprocal space computations, our method achieves the same computational complexity, $\mathrm{O}(N \log N)$, as the traditional 3D Ewald technique. These improvements provide a more efficient framework for simulating 2D periodic systems, significantly reducing computational expenses. As shown in Table 1, a typical MD simulation of 1 ns with 2D periodicity with the new method is approximately 2.5 times faster.

By maintaining accuracy without compromising computational speed, our method offers a practical and efficient framework for large-scale molecular simulations, which will have implications for simulating 2D periodic systems found in surface science, material interfaces, and thin films.

| Time (sec) → | Real | Reciprocal (k $\neq$ 0) | Reciprocal (k = 0) | Total (sec) | Time for 1 ns Simulations (days) |
|---|---|---|---|---|---|
| 3D Ewald (SPME)[4] | 1.421 | 0.047 |  | 1.467 | 16.98 |
| 2D Ewald [5] | 0.881 | 1.449 | 0.295 | 2.625 | 30.39 |
| Our Work | 0.881 | 0.097 |  | 0.978 | 11.32 |

Table 1: Computational time breakdown for a 1 ns MD simulation of a 10,000-atom system

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# Regenerable Fe-Ag-CNF Catalyst for Industrial Wastewater Treatment via Catalytic Wet Air Oxidation

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## Abstract

A bimetallic Fe-Ag tipped carbon nanofiber supported on activated carbonized beads (Fe-Ag-CNF/ACB) catalyst was developed for continuous catalytic wet air oxidation (cWAO) of industrial wastewater. The catalyst was synthesized through a multi-step process, starting with the formation of bimetallic beads via suspension polymerization of phenol-formaldehyde co-polymeric beads in situ doped with Fe and Ag salts, followed by carbonization, steam activation, and acetylene chemical vapor deposition. Fe-Ag-CNF/ACB has a surface area of 465 $m^2/g$ and a pore volume of 0.314 cc/g. The cWAO process operated at 244 °C and 27 bar oxygen pressure, achieving 99% degradation of organic pollutants. Initial experiments at a 1 cc/min water flow rate required 25 g of catalyst, sustaining continuous pollutant degradation for 12 h. Scale-up trials successfully increased the flow rate to 5 cc/min with a proportional catalyst amount of 125 g. A linear correlation between catalyst quantity and wastewater treatment efficiency confirmed that 9.77 g of catalyst was required to treat 1 L of wastewater. Spent catalyst was in situ regenerated through a sequential process involving acid-acetone-water washing, steam activation, $H_2$ reduction, and $KMnO_4$ impregnation. The catalyst has a lifespan of one fresh cycle plus four regeneration cycles. The findings highlight the potential of Fe-Ag-CNF/ACB catalyst for efficient, scalable, and sustainable wastewater treatment through continuous cWAO operation.

**Keywords:** Catalytic wet air oxidation; carbon nanofibers; activated carbonized beads; continuous operation; pollutant degradation.

# Interval Hessian-based Optimization Algorithm

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## Abstract

Second-order optimization algorithms based on the Hessian of the objective function have been proven to achieve a faster convergence rate than the first-order methods. Additionally, these algorithms typically require fewer iterations to converge. However, their application to large-scale nonconvex problems is hindered due to the computational cost associated with three major operations required at every iteration: (1) Hessian evaluation, (2) Hessian matrix inversion to find the search direction, and (3) modifying the Hessian matrix to ensure its positive-definiteness so that the search direction is descent.

Accordingly, we propose a new search direction based on interval Hessian and incorporate it in a line-search framework to find a local minimum of unconstrained nonconvex optimization problems. **Step 1** We define $p$ as the index corresponding to the Hessian update and $k$ corresponding to the iterate update. **Step 2** At p, we define an interval region $[x_p^l, x_p^u]$ around the current iterate $x_p$ and estimate an interval Hessian $[\nabla^2 f_p]$. **Step 3** We then calculate a positive-definite approximation $H_p = \nabla^2 f_p + \lambda_p$, where $\lambda_p$ is the estimated lower bound of the minimum eigenvalue obtained using Gerschgorin, E-Matrix, and Mori-Kokame methods. The matrix $H_p$ can be viewed as the Hessian of the $\alpha BB$ convex underestimator (Adjiman et al., 1998). **Step 4** The search direction is determined by $H_p^{-1} \nabla f_k$, and **Step 5** the new iterate $x_{k+1}$ is computed using Armijo conditions. **Step 6** If $||\nabla f_k|| < \epsilon$, then terminate the algorithm, otherwise, updated the index $k \leftarrow k+1$. If $x_{k+1} \in [x_p^l, x_p^u]$, then go to step 4, otherwise $p \leftarrow p+1$ and go to step 2. Note that interval Hessian is computed only once per interval, significantly reducing computational cost.

The novelty of the algorithm is that, unlike traditional second-order methods, we avoid performing expensive operations at all iterations. Specifically, for the iterations with $x_k \in [x_p^l, x_p^u]$, we compute the Hessian only once, and the search direction is obtained by matrix-vector multiplication. On the other hand, Hessian is computed at every iteration in Newton's method and finding the search direction requires $\mathcal{O}(n^3)$ operations. We apply our algorithm on a set of 210 problems and show that our method converges to a local minimum for 70% problems for 0.1 as interval size using the Mori and Kokame Method.

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# Abstracts for Poster Presentations

RSD2025 ChE@IITK

# Evaluating Dehydrogenase Inhibitors against Human CtBP1: Docking Studies and Molecular Dynamics Simulations

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## Abstract

Human C-terminal Binding Protein 1 (CtBP1) is an important transcriptional repressor and its overexpression is associated with several human diseases, indicating that it can be a target for drug therapy. We performed molecular docking analyses focusing on the four known dehydrogenase inhibitors Disulfiram, Enoxolone, Mycophenolic Acid and Leflunomide for their binding affinities and interaction profiles within CtBP1 in monomeric and dimeric states.

Due to the unavailability of the CtBP1 dimer structure, we generated its three-dimensional model using AlphaFold. Docking studies performed using AutoDock Vina revealed that among the tested inhibitors, Enoxolone exhibited the highest binding affinity (most favourable) towards both CtBP1 monomer and dimer. Subsequent analysis indicated that specific residues in CtBP1 are critical in stabilizing the interactions between the CtBP1 protein and the Enoxolone compound.

Currently, Molecular Dynamics (MD) simulations are underway to explore the conformational stability of CtBP1-Enoxolone complex. Root Mean Square Fluctuation (RMSF), Radius of Gyration (Rg), Interaction Energy, Ligand-Protein Distance are among the parameters being analysed. These detailed analyses will yield insights into the structural dynamics and stability of Enoxolone-induced CtBP1 complexes, possibly informing future inhibitor optimization studies against CtBP1-driven disease.

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# Robust Flowsheet Synthesis for Ethyl Acetate, Methanol and Water Separation

Kartavya Maurya[1], Aayush Gupta[1], Prakhar Srivastava[1] and Nitin Kaistha[1]

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## Abstract

Ethyl acetate (EtAc) and methanol (MeOH) are widely used industrial solvents (Shiyu et al., 2014), generating waste streams that necessitate recovery due to stringent environmental regulations. However, the presence of a homogeneous EtAc-MeOH azeotrope and a heterogeneous EtAc-water azeotrope imposes distillation boundaries, making conventional separation techniques infeasible. The challenge is further compounded by the inherent variability in industrial waste solvent compositions, which can render fixed flowsheet designs ineffective under different operating conditions.

This study proposes a robust and composition-independent flowsheet for the complete separation of EtAc-MeOH-water waste streams, ensuring process feasibility across a wide range of feed compositions. The key innovation lies in the integration of a liquid-liquid extractor (LLX) using recycled water as the solvent, which enables selective phase separation. For sufficiently high water addition, the raffinate composition aligns with the EtAc-water edge, facilitating its separation in the EtAc-rich distillation region. The recovered EtAc is obtained as a high-purity product, while the aqueous phase undergoes stripping and further distillation to yield pure MeOH and water, with the latter being partially recycled to the LLX for solvent extraction continuity.

The robustness of the proposed flowsheet is validated through process simulations for equimolar, EtAc-rich, MeOH-rich, and water-rich waste compositions. The results confirm its adaptability, demonstrating consistent separation performance across varying feed conditions. This approach enhances process flexibility, economic feasibility, and sustainability, offering a viable solution for industrial-scale solvent recovery.

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# Control Strategy for the Intensified Compact Azeotropic Process for EtAc-MeOH-Water Separation

Prakhar Srivastav[1], Mounish Kumar[1], Aayush Gupta[1] and Nitin Kaistha[1]

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## Abstract

Aqueous waste streams containing organic solvents like ethyl acetate (EtAc) and methanol (MeOH) are common in pharmaceutical manufacturing (Constable, Jimenez-Gonzalez, and Henderson, 2007). Efficient separation of these solvents is crucial for environmental compliance, resource recovery, and sustainable processing. However, the presence of azeotropes—homogeneous EtAc-MeOH and heterogeneous EtAc-water makes conventional distillation challenging.

Several advanced techniques have been proposed in the literature to separate these dilute mixtures of EtAc, MeOH, and water. Recently, (Srivastava, Gupta, and Kaistha, 2024) developed an alternate flowsheet compared to the existing best flowsheet in the literature. They utilized pressure sensitivity and liquid-liquid phase separation to improve the efficiency. The process contains a decanter and high pressure coloumn and a low-pressure dividing wall column. This was further optimized into the heat-integrated compact distillation(HI-CD) system, which included external heat exchangers for energy savings. Energy efficiency was further improved through the incorporation of vapor recompression-driven reboiling and process-to-process heat exchange, ultimately yielding the hybrid-CD process.

While these systems have been well studied in steady-state conditions, their behavior under dynamic operating conditions and their control strategies have not been explored in detail,presenting a critical research gap. This study focuses on the dynamic simulation and control of the HI-CD and Hybrid-CD processes. A structured dynamic control strategy is developed to ensure operational stability. Initially, a control structure (CS1) was proposed, where the fresh feed to the decanter acted as the throughput manipulator (TPM). However, dynamic simulations revealed a critical issue: -2% composition change in the feed caused the organic level controller in the decanter to saturate, leading to ineffective separation. Additionally, a 20% increase in TPM resulted in flooding in Column C1, significantly affecting separation efficiency and causing instability.

To address these challenges, an improved control structure (CS2) was developed, selecting the total feed to the liquid-liquid separator as the TPM. This adjustment provided greater flexibility to manage fluctuations in both feed rate and composition, ensuring stable and efficient process performance without column flooding. Simulation results confirm that CS2 effectively maintains process stability and product quality even under disturbances. These findings underscore the potential of heat-integrated and vapor-recompressed distillation systems for energy-efficient solvent recovery and industrial applications.

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# Elucidating the Catalytic Activity of Doped Molten Bismuth and Bismuth Trichloride Systems: A DFT Study

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## Abstract

Molten salts are ionic solvents consisting of electrically charged species that are stable at elevated temperatures. The use of molten catalysts in reaction media allows the easy separation of carbon from the surface, thereby offering a remedy to the problem of active site deactivation in solid catalysts. Bismuth and its derivatives are known as "green reagents" because of their safe use that does not pose a hazard to the environment. Bismuth chloride ($BiCl_3$) salt with poor deshielding from 4f electrons displays Lewis acidity, making it a catalyst for reactions such as alcohol chlorination, Friedel-Crafts alkylation, etc. An early solubility study of the $BiCl_3$ (A) - Bi (B) system suggests limited mixing at low temperatures due to the formation of solid Bi–Cl subhalides, which increases beyond the eutectic point, reaching complete miscibility past a consolute temperature of 780 °C. Practically nothing is known about the catalytic behavior of this system. This study models doped $BiCl_3$–Bi molten systems to explore their catalytic activity in the activation of $H_2$, $CO_2$, and $CH_4$. Activation of all these molecules is rate-limited by their decomposition steps. We have modeled 40$BiCl_3$ (pure salt), 40$BiCl_3$-4Bi (10% Bi-doped salt), 100Bi (pure metal), and 100Bi-4$BiCl_3$ (4% $BiCl_3$-doped metal), 60Bi-15$BiCl_3$ (25% $BiCl_3$-doped metal) as various compositions of liquid slabs containing molten $BiCl_3$ salt and Bi metal. In salt-rich systems, catalysis of $H_2$ and $CO_2$ dissociation reactions were investigated, whereas in metal-rich systems, the focus was on the dissociation of $CH_4$.

All periodic spin-polarized DFT calculations and ab initio molecular dynamics (AIMD) simulations were performed using CP2K software package. In the NVT ensemble, AIMD simulations were conducted at temperatures of 300 °C and 1000 °C for systems rich in salt and metal, respectively. Using the climbing-image nudged elastic band (CI-NEB) method, the activation energy barriers of methane dissociation were calculated.

**$BiCl_3$ rich-melt**: The addition of 10 mol% Bi leads to the formation of dimers and trimers of Bi ions, having Bi in the valency of +2 and +1. It is envisaged that these under-valence Bi ions may be active for catalysis. AIMD calculations were performed to determine the dissociation energies of $H_2$ and $CO_2$ in the salt-rich melt. The cumulative mean energy from AIMD runs indicates that dissociating $H_2$ into 2H and $CO_2$ into CO + O is thermodynamically more favorable by 223 kJ/mol and 289 kJ/mol, respectively, in doped bismuth chloride compared to undoped bismuth chloride.

**Bi rich-melt**: On doping molten Bi with 4-25 mol% $BiCl_3$ salt, we find that barriers for methane dissociation are reduced by ~100-170 kJ/mol (see Figure 1). At high temperatures,

increased $BiCl_3$ doping may lead to HCl gas formation, which can reduce $BiCl_3$ to Bi metal. However, recycling HCl back into the reactor can help regenerate $BiCl_3$, sustaining the catalyst.

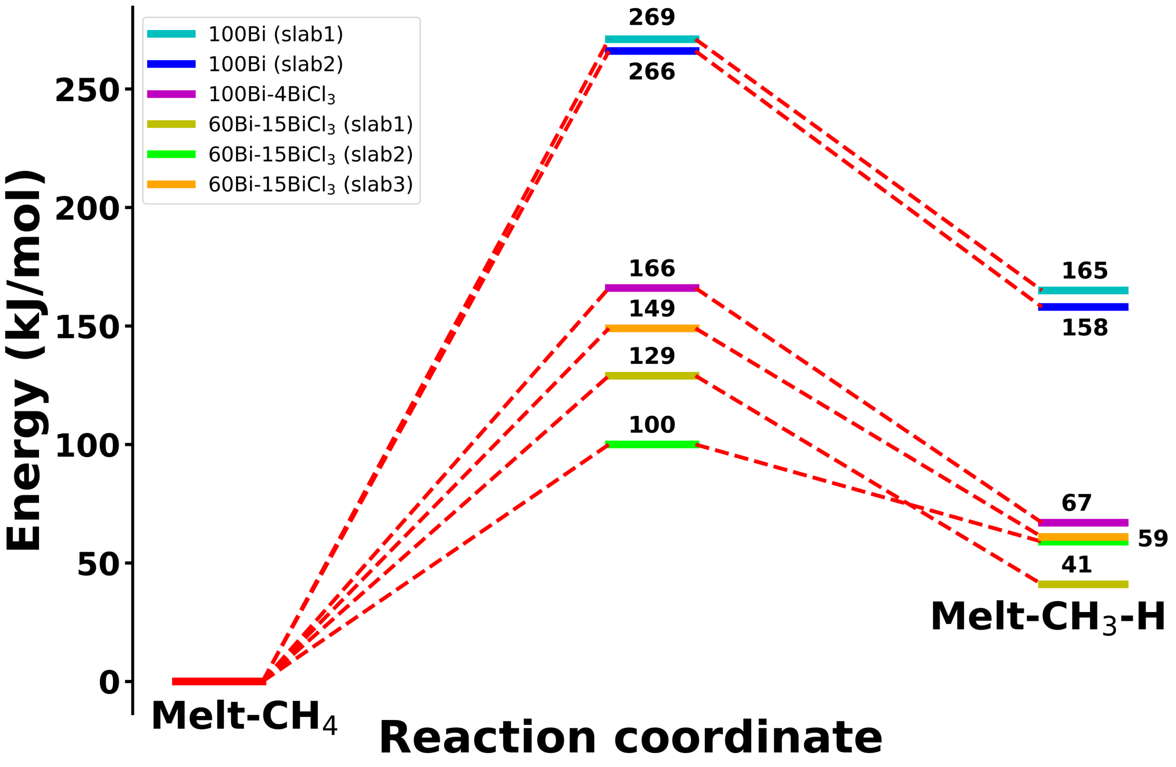

Figure 1: Potential energy pathways for methane dissociation on molten slabs of pure molten Bi and $BiCl_3$-doped molten Bi slabs in various compositions. Here, “Melt” denotes the respective molten system. The adsorption complex is represented with a “-” symbol. For example, “Melt-$CH_3$-H” represents adsorption of $CH_3$ and H on molten.

# Role of Carbon species in Pyrolysis of Methane: Insights from molten In-Sn and In-Ni

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## Abstract

Methane, a highly potent greenhouse gas (GHG), can be efficiently converted via pyrolysis into solid carbon and pure hydrogen—a valuable industrial precursor essential for producing methanol, ammonia, and various other chemicals. However, conventional solid catalysts used in this process often suffer from deactivation due to the accumulation of carbon deposits on their surfaces, adversely affecting their catalytic performance and longevity. Producing hydrogen without generating $CO_2$ emissions presents a major challenge. Among the various clean technologies utilizing natural gas, methane pyrolysis in molten catalytic systems has attracted considerable attention due to its unique advantages, including resistance to catalytic deactivation and superior heat transfer characteristics, making it a promising approach for sustainable hydrogen. It is shown previously that In-based alloys, in particular, demonstrate superior efficiency in converting $CO_2$ and $CH_4$ compared to alloys based on Sn and Ge. This study presents a comparative analysis to investigate the influence of accumulated carbon species on the surface of molten In-Sn and In-Ni alloys in facilitating methane pyrolysis. Our findings elucidate the role of carbon on the surface characteristics of the molten catalyst and its influence on the reaction pathway.

The nature of carbon species was investigated by introducing one or more carbon atoms into the simulation cell of molten In-Sn and In-Ni alloys. AIMD simulations revealed that, in the In-Sn system, carbon atoms preferentially reside on the surface which is supported by mean energy calculations, showing that the surface position is energetically more stable than the bulk position. In contrast, in the In-Ni system, the carbon atoms favored the sub-surface or bulk positions, as these configurations exhibited comparable energy stability. Figure 1 illustrates the average atomic distribution of In and Sn (or Ni) within the melt in the presence of 10 carbon atoms. For the In-Sn system, most of the carbon atoms segregate to the surface, forming dimers, whereas, for the In-Ni system, the carbon atoms predominantly diffuse in the sub-surface region. For the In-Sn system, surface carbon atoms were found to have, on an average, $\sim 2$ Sn, $\sim 1$ In, and $\sim 1$ C atoms as neighbors within the first coordination shell, indicating that carbon has more affinity for Sn than In. Furthermore, the presence of these carbon atoms leads to an increase in the Sn/In ratio at the surface, which will change the reactivity of the surface melt. Similarly, in the case of the In-Ni system, sub-surface carbon atoms were observed to have an average of $\sim 5$ Ni atoms as their nearest neighbors, indicating stronger affinity for Ni, which

tends to pull Ni atoms toward the sub-surface region. This results in an increased Ni/In ratio in this region compared to the distribution observed in the absence of carbon. Variations in the mean Bader charge of In and Sn with respect to time indicate that, at any given moment, tin (Sn) atoms typically exhibit a negative charge, while indium (In) atoms maintain a positive charge. However, when carbon atoms segregate to the surface, the average charge on Sn atoms becomes positive at any given time. Without carbon, the surface In and Sn atoms already exhibit more positive average charges than their bulk counterparts. Interestingly, with surface-segregated carbon, the average charge on In and Sn in the affected region further increases, making them even more positively charged. Likewise, in the In-Ni system with carbon atoms, the average charge on Ni in the carbon-segregated region becomes less negative. Given the altered reactivity of the surface melt in the presence of these carbon species, we investigated the activation energy barriers for $CH_4$ dissociation on both these molten alloys and observed no significant variation in the barriers compared to the system without the presence of carbon species.

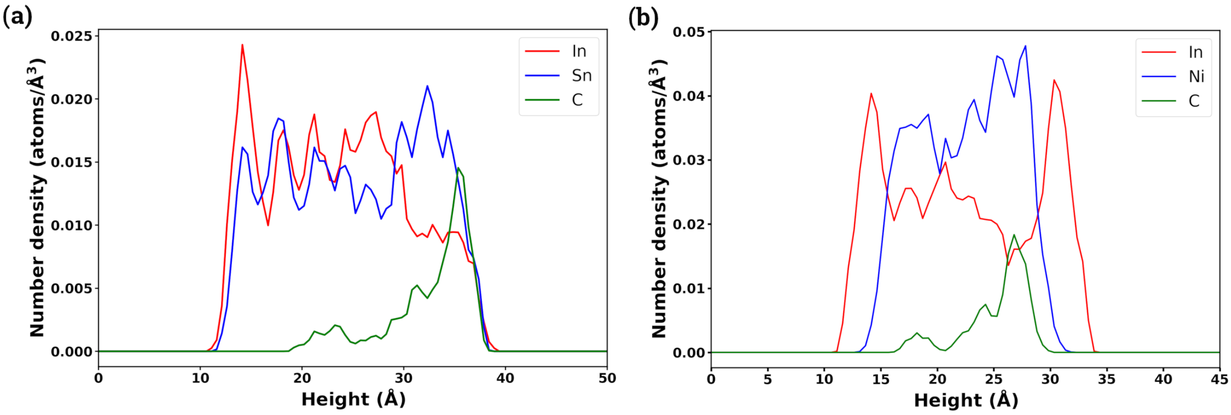

Figure 1: Atomic distribution profiles of the molten slab system: (a) average number density of In, Sn and C atoms, and (b) average number density of In, Ni and C atoms, plotted as a function of height within the liquid film.

# Theoretical investigation of methane pyrolysis in vapor and molten Magnesium-based catalysts

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## Abstract

In response to the growing energy demand and the need for sustainable and environmentally friendly energy sources, hydrogen fuel has emerged as a viable alternative. While steam reforming of natural gas and light hydrocarbons is an efficient industrial method for hydrogen production, it also generates carbon oxides (CO and $CO_2$), which are undesirable. $CH_4$ pyrolysis using molten metal catalysts has garnered attention due to their notable advantages, including the production of high purity $H_2$ devoid of carbon oxides (CO and $CO_2$), absence of catalytic deactivation issues, enhanced heat transfer capabilities, and easy carbon removal. In this work, we have investigated molten and gas-phase Mg, Zn and Mg-Zn alloy for $CH_4$ pyrolysis using quantum chemical calculations. Previous studies have demonstrated that molten Mg is an effective catalyst for methane dissociation. Zn is chemically similar to Mg in that both elements primarily exhibit a +2 oxidation state and possess comparable ionic sizes. However, both Mg and Zn have high vapor pressures. Therefore, Mg and Zn vapors are likely to be present both above the melt and inside the $CH_4$ bubble. Consequently, we have examined the catalysis of the $CH_4$ pyrolysis process in both the vapor and liquid phases. Our findings indicate that gas-phase pyrolysis is hindered by high activation barriers (338 kJ/mol for monomeric Mg and 376 kJ/mol for monomeric Zn atoms) for C-H bond dissociation step, which is considered to be the rate-limiting step. Whereas, the liquid surfaces of Mg, Zn, and Mg-Zn alloy exhibit catalytic properties conducive to $CH_4$ pyrolysis, with activation barriers ranging from 165-181 kJ/mol for Mg, 138-192 kJ/mol for Zn, and 177-190 kJ/mol for the Mg-Zn alloy. The activation energies for these systems were found to be significantly lower than those of uncatalyzed gas-phase $CH_4$ pyrolysis and are comparable to the most active molten metal catalysts reported to date, highlighting the catalytic efficiency of these liquid systems. Carbon byproduct behavior varies among these systems. In molten Mg, carbon tends to migrate to the surface, facilitating easier separation. Conversely, in molten Zn and the Mg-Zn alloy, carbon is drawn into the bulk, increasing the risk of metallic contamination. Our findings indicate that while molten Mg and Zn exhibit competitive catalytic performance for $CH_4$ pyrolysis, alloying these metals offers no substantial catalytic advantage and may pose additional complexities related to carbon separation.

# Molybdena as a promoter for propane dehydrogenation (PDH) reaction over $ZrO_2$ supported vanadia catalyst: An experimental + DFT study

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## Abstract

Supported vanadia oxide serves as a promising catalyst for non-oxidative propane dehydrogenation (PDH) reaction due to its higher conversion rates, enhanced propylene selectivity and improved activity. However, there are only a limited number of studies that have explored the promotional effect of adding a secondary inactive metal oxide on the overall conversion of propane to propylene via the direct dehydrogenation. In this study, we have conducted experiments along with density functional theory (DFT) calculations to investigate the role of molybena (which is itself inactive for PDH) as a promoter for propane dehydrogenation reaction. Raman spectroscopy and XPS results of freshly calcined catalysts show that both molybdena and vanadia are present as isolated moieties, and even when these moieties are simultaneously present, there is no interaction between them. Next, we investigated the reactivity of propane dehydrogenation on the different metal oxide catalysts as a function of temperature and also as a function of time-on-steam(TOS). Our experimental results on PDH reactivity indicate that the presence of molybdena as a promoter leads to a 4-5% enhancement in both the conversion of propane and yield of propylene. To investigate the underlying reasons for this enhancement, we performed spin polarized DFT simulations. Oxygen vacancy formation energy, propane adsorption and dissociation energies on isolated $VO_x$ and $MoO_y$ moieties (also when they are present together) and two hydrogen (2H) abstraction energies were some of the parameters that were studied to understand the promotional behaviour shown by the molybedena moiety. Our results shows that the addition of molybdena moiety has no discernible effect on the oxygen vacancy formation energies of vanadia and also on the adsorption and dissociation energies of propane. However, addition of molybdena together with the vanadia moiety significantly reduces (by $\sim$ 1.2 eV) the energy required for the abstraction of the second hydrogen, thereby showcasing its promotional effect. Further, by applying the Brønsted-Evans-Polanyi relationship it can be inferred that the presence of secondary metal oxide may reduce the energy barrier required for the abstraction of the second hydrogen which explains the enhancement observed during PDH of the $VO_x$-$MoO_y/ZrO_2$ catalyst.

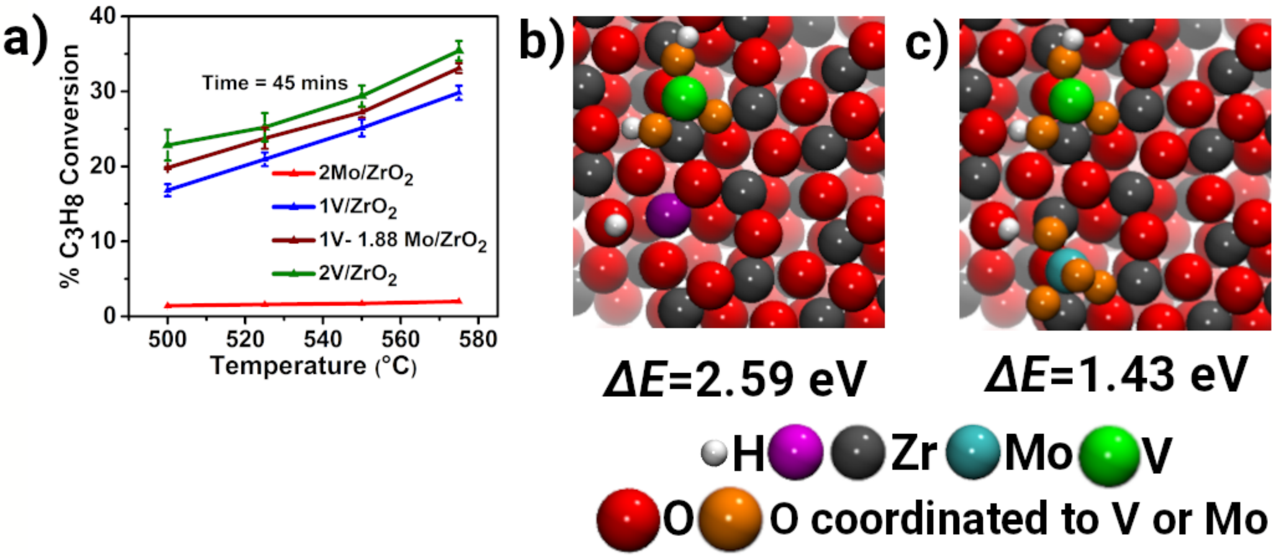

Figure 1: **Left panel**: Reactivity study of propane over different metal oxide catalysts supported on $ZrO_2$ as a function of temperature. **a)** Conversion of propane for different catalysts as a function of different reaction temperature at a TOS of 45 min. **Right panel**: Configuration of adsorbed hydrogens on supported moieties. **b)** Adsorption of 2H when only single isolated $VO_x(H)$ moiety is present. **c)** Adsorption of 2H when $MoO_y$ moiety is present along with the $VO_x(H)$ moiety. $\Delta E$ is the energy of adsorption of two hydrogen.

# Diffusiophoretic transport of colloids in microporous confinements

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## Abstract

The transport of colloids in dead-end microchannels is pivotal to numerous applications, including drug delivery, textile cleaning, anti-bacterial clothing, and underground oil and gas recovery. Traditional reliance on Brownian dynamics for understanding the transport of microscale colloidal particles (into or out of the pores) is inefficient. We theoretically investigate the potential of diffusiophoresis — a phenomenon where colloidal particles move in response to solute concentration gradients without the application of any external force — and to enhance this transport by applying varying external chemical gradients.

Through a comprehensive numerical model of colloidal transport via diffusiophoretic injection and withdrawal into dead-end channels, our results affirm a significant enhancement. The particle injection/withdrawal rates increase by orders of magnitude compared to Brownian diffusion alone. To evaluate the effectiveness of this mechanism, we introduce effectiveness and penetration depth as key performance metrics. Furthermore, we find that this rapid enhancement is characterised by propagating fronts whose behaviour is highly sensitive to ambient concentrations. To emulate the aforementioned applications, we analyse the cases of ambient concentration varying over a time scale that is comparable to the diffusiophoretic persistence. Our findings underscore the potential of leveraging solute gradients to substantially improve the efficiency of colloidal transport in dead-end channels.

**Keywords:** Diffusiophoresis, Dead-end pore.

# Rheology of Wax-Based Oleogels

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## Abstract

Oleogels are materials formed by self-assembly of gelator molecules within a liquid oil phase. They have gained significant interest due to their unique properties and diverse applications in food science, pharmaceuticals, and cosmetics. It has been observed that oleogels undergo a sol-gel transition upon a decrease in temperature, transforming from a free-flowing liquid (sol) to a structured gel network.

In this work, we have taken corn oil as the liquid phase and prepared oleogels by varying the concentration of beeswax. We study the change in frequency dependence of dynamic moduli at different temperatures while cooling and heating. As the temperature decreases, we observe all the rheological signals of the sol-gel transition, wherein the loss tangent ($\tan\delta$) or loss modulus becomes independent of the angular frequency at the critical gel point. We study how changing the beeswax concentration as well as the rate of cooling alters the critical gel state in oleogels.

# Superhydrophobic coatings for oil-water separation

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## Abstract

Oil-water separation is a critical process in various industries, including petroleum refining, wastewater treatment, and environmental remediation. The presence of oil contaminants in water sources poses severe environmental and economic challenges, necessitating efficient separation technologies. Traditional separation methods, such as gravity settling, skimming, and chemical coagulation, are often inefficient and energy-intensive, especially for stable oil-water emulsions.

Recent advancements in materials science have led to the development of superhydrophobic and superoleophilic surfaces, which can selectively repel water while absorbing oil. These materials, inspired by natural phenomena like the lotus leaf effect, offer promising solutions for high-efficiency oil-water separation. Membrane-based separation, nanomaterials, and functional coatings have also gained significant attention due to their reusability, scalability, and environmental friendliness. Our research focuses on superhydrophobic coatings derived from agricultural waste, rice husks, and different polydimethylsiloxane (PDMS) fractions. Developed coatings showed the presence of hierarchical structures with nanoscale protrusions. The surface morphology of the coatings was significantly influenced by the PDMS content with a roughness factor following an inverse correlation. This coating applied to fabrics can contribute to this field by developing robust, durable, and cost-effective solutions for oil-water separation. Integrating advanced surface engineering techniques can enhance separation efficiency, self-cleaning properties, and long-term performance.

The synthesized materials have a superhydrophobic nature with a water contact angle greater than (WCA)$>150^o$ and a low sliding angle ($<10^\circ$), indicating easy water droplet roll-off. Coating demonstrated self-cleaning ability by rolling off contaminants with water droplets. The formed coated fabric material was Successfully employed to selectively mop up various oils like sunflower oil, engine oil, and diesel from the water surface. After performing more than 30 cycles with various oil-water mixtures (e.g., crude oil, diesel, vegetable oil), the separation efficiency retained over $>95\%$. Retained superhydrophobicity after multiple separation cycles (30+ cycles) by maintaining the contact angle $>150^o$. To check performance, the coating was subjected to harsh environmental conditions, such as acidic, basic, and saline environments. After the tests, the coating retained superhydrophobic behavior. SEM analysis of coating shows a rough hierarchical structure enhancing water repellency. EDS/XPS confirms the presence of low-surface-energy materials (e.g., silica or polymeric coatings). The coatings are easy to clean after separation while maintaining the ability to separate oil/water.

Keywords: superhydrophobic; oil/water separation; self-cleaning; Durable

# Repurposing a 3D Printer as a Capillary Rheometer for Printability Analysis

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## Abstract

Extrusion-based 3D printing is an additive manufacturing technique that constructs structures layer by layer by extruding material through a narrow capillary. The process involves multiple stages, including extrusion, ink deposition, and solidification, each of which is influenced by various printing parameters such as temperature, pressure, ink flow rate, capillary diameter, and capillary length. Determining these parameters requires thorough rheological characterization. Rheological properties, which significantly impact both the printing process and the quality of the printed structures, are typically analyzed using rotational and capillary rheometers. A capillary rheometer operates by forcing material through a narrow capillary tube under controlled conditions of pressure, temperature, or flow rate. It provides valuable insight into the phenomena occurring inside the capillary, replicating actual scenarios encountered during extrusion-based 3D printing. In this work, a 3D printer is repurposed to function as a capillary rheometer. This work presents the results of Pluronics F-127 chosen as 3D printable ink. The rheological properties such as viscosity and yield stress (minimum stress or pressure required to extrude the ink) have been obtained from 3D printer. Additionally, an optimal range of temperature and pressure for achieving the best 3D print has been mentioned. The printability parameter has been calculated to determine the best-printed structure.

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# Influence of Substrate Stiffness and Marangoni Flow on Biofilm Spreading

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## Abstract

Bacterial swarming and biofilm formation are multicellular phenomena through which various microbial species evolve on water-permeable substrates. These water-permeable substrates are generally considered to be soft viscoelastic materials. The stiffness of the substrate influences colony morphology and spreading dynamics.

In the literature, biofilm spreading is primarily attributed to nutrient availability in the substrate and Marangoni flow due to surface tension gradients at the biofilm interface [3]. Typically, the substrate is considered solid and non-deforming. However, studies suggest that increasing substrate stiffness accelerates biofilm growth, whereas a softer gel slows down the spreading rate [1]. We model this phenomenon using a two-phase system, where the soft solid substrate is represented by the Kelvin-Voigt model. In our model, we assume an excess supply of nutrients and consider osmotic influx due to the osmotic field created by bacteria at the biofilm-substrate interface [2]. We assume that osmotic water transfer from the substrate to the colony does not alter the substrate structure, meaning that despite the transport of the aqueous phase, the substrate remains structurally unaffected. Our results indicate that increasing substrate softness leads to a slower colony growth rate, which aligns with experimental observations [1].

We also investigate the Marangoni effect on colony morphology and find that Marangoni flow enhances colony spreading [2]. However, Marangoni flow is primarily studied in the solid substrate regime. Our simulations show that our results qualitatively match experimental findings [1, 3].

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# Driven Translocation of a Polymer Chain: Theory and Simulation

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## Abstract

A comprehensive understanding of the kinetics of polymer translocation is of great significance for applications in nanotechnology and health care. The kinetics of this stochastic process has been described in terms of a mean-first-passage-time for the entire polymer chain, initially just inside the nanopore, to pass through the nanopore. This time directly maps to an experimentally measured quantity, *viz.* dwell-time. Equilibrium and non-equilibrium theories have been suggested by researchers to model these kinetics. Specifically, assuming quasi-equilibrium, the Fokker-Planck equation describes the kinetics as a drift-diffusion on a 1-D collective variable. In addition to the key assumption of quasi-equilibrium, the equation requires an accurate estimate of the variation in free energy along the collective variable.

Here, we present a direct comparison between the dwell-time distribution obtained using Langevin dynamics simulation of a charged polymer translocating through a nanopore under the action of an electric field, and the mean-first-passage-time calculated using the Fokker-Planck equation. A continuous and differentiable collective variable is defined to denote the progress of translocation. Metadynamics simulation is used to obtain the free energy landscape along this collective variable.

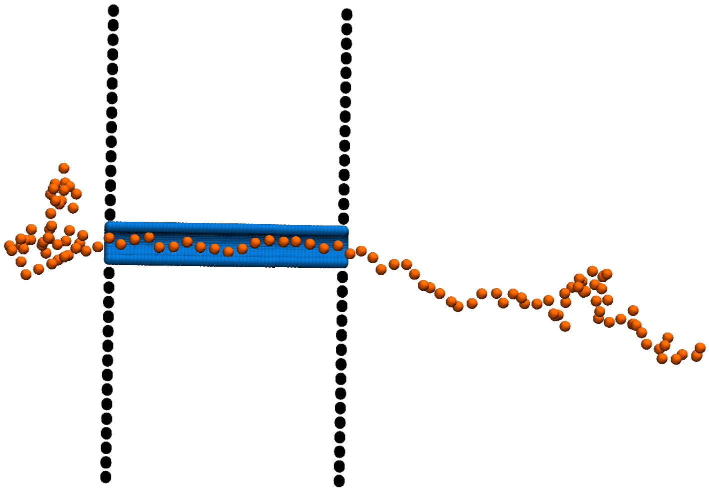

Figure 1: Polymer chain translocating through a nanopore.

# Emergence of Order in Chemically Active Droplets: Temporal Dynamics and Collective Behavior

Sobiya Ashraf[1], Pawan Kumar[1], Prateek Dwivedi[1], Frédéric Blanc[2], Dipin Pillai[1] and Rahul Mangal[1]

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[2]*Institut de Physique de Nice, CNRS Université Côte d'Azur, France*

## Abstract

Collective behaviors such as swarming, chemical signaling, and clustering are fundamental to biological microorganisms, enabling hierarchical colony formation, coordinated motion, and enhanced nutrient accessibility—crucial for their survival. Over the past few decades, extensive research has been dedicated to unraveling the mechanisms underlying these diverse collective patterns through experimental model systems. Among these, active droplets have emerged as valuable synthetic analogs, effectively replicating key biological attributes and serving as ideal platforms for investigating collective phenomena. This research explores the collective behavior of 4-Cyano-4'-pentyl-biphenyl (5CB) oil droplets across varying Péclet ($Pe$) numbers. At high $Pe$, droplets exhibit a pusher mode of propulsion and form dynamic chain-like patterns. Decreasing $Pe$ enhances repulsive interactions among droplets, resulting in the inhibition of clustering. In the low $Pe$ regime, their repulsive interactions predominated by chemical field lead to the emergence of an ordered structure. Furthermore, we illustrate how active droplets efficiently navigate within a soft structured environment. These findings contribute to our comprehension of self-organized phenomena in active matter systems and provide insights for designing strategies for controlled locomotion in intricate fluidic environments [1].

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# Deep Eutectic Solvent-Based Cured Emulsion Beads for $CO_2$ Capture

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## Abstract

Deep Eutectic solvents (DESs) have gained significant recognition as biodegradable and non-toxic solvents and find a wide range of applications. In this study, DES serves to capture $CO_2$, as a potential green alternative to amine-based solvents due to their high $CO_2$ absorption capacity, high regenerative capacity, and low volatility.

The high viscosity, leading to low mass transfer rates, negatively impacts the absorption process, so a Cured Emulsion Bead (CEB) system similar to Einloft and Bernard, 2020 was synthesized having a large interfacial area and incorporating DES instead of directly using it. Stable DES-in-Oil Pickering emulsions are formed with functionalized $TiO_2$ nanoparticles acting as emulsifiers. An increase in the concentration of the emulsifier leads to a decrease in the droplet size and an increase in the emulsion stability. Emulsions comprising of various DES combinations such as Choline chloride and Urea, Choline chloride and Glycerol, L-arginine and Glycerol, with high proportion of DES have been explored to improve their stability for greater loading in a $CO_2$ permeable polymeric shell.

$CO_2$ absorption analysis of these CEBs' gave valuable insights about their carbon-capturing capacities.

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# Use of Polyglycerol sebacate (PGS) as an alternative to Polydimethylsiloxane (PDMS) for making microfluidic devices

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## Abstract

PDMS (polydimethylsiloxane) is optically transparent, biocompatible, easily crosslinkable, moldable, flexible, benign material of low surface energy that allows for different surface modification strategies. Therefore, it has been used extensively for making microfluidic devices suitable for a large variety of applications: biomedical diagnostics, chemical synthesis, chemical sensors and so on. However, PDMS is non-biodegradable, expensive, and scarce in many places. Hence there is a need for finding an alternative material that will incorporate most characteristics of PDMS but allows for easy degradation after its application is over. Here we have presented a novel strategy in which Poly (glycerol sebacate) (PGS), a nearly transparent thermoset elastomer prepared by polycondensation reaction of equimolar quantities of sebacic acid and glycerol, has been used as a platform for making microfluidic channels. PGS is a biocompatible, biodegradable, non-edible vegetable oil based polymeric material which we have shown can be made into micro-channels of a variety of shapes, sizes and complexities. In particular, we have used aqueous solution of NaOH, which is known to degrade many biomaterials, in a controlled manner to etch out channels of different types: straight and spiral, straight with curved extension and different channels within a channel. We have systematically varied the crosslinking density, NaOH concentration, etching time to optimize the process. FTIR and Raman spectroscopy shows that PGS is polar in nature. Therefore, we have also explored the possibility of surface functionalization of PGS by making use of hydroxyl groups on its surface, which makes it suitable for both dry and wet applications, e.g. adhesion and wetting. An example of surface modification is coating with mussel secretive protein: Dopamine, a small molecule which has been widely used for attachment to wet surfaces via its catechol and amine groups. We have coated PGS with a layer of polydopamine, a self-polymerized form of dopamine, and subsequently characterized these coated samples and performed adhesion tests on them.

# $Ni/Al_2O_3$ Catalysts for Efficient Ammonia Decomposition: Effect of Metal Loading and Fe Promotion

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## Abstract

Hydrogen has emerged as a promising fuel for the future due to the worldwide commitment to decarbonization. Nevertheless, the storage and transportation of hydrogen continue to be significant challenges in its technical advancement. The process of catalytically decomposing ammonia to generate on-site hydrogen is aimed at overcoming these difficulties. Ruthenium (Ru) based catalysts demonstrate excellent catalytic performance on various metal oxide supports. However, the high cost of Ru limits large-scale industrial applications. In contrast, transition metal-based catalysts (Ni, Co, and Fe) offer a more cost-effective alternative. Among them, nickel stands out as the most catalytically active and widely studied metal for industrial processes (Ganley, 2004). Here, our initial focus is to optimize the Ni-based catalysts supported on alumina by varying the Ni loading. Subsequently, the effect of Fe is explored by substituting Ni with Fe in the bimetallic catalysts. To achieve this objective, several $Ni/Al_2O_3$ catalysts are synthesized and finally calcined at 850 $^oC$ for 5 h to take advantage of the metal-support interaction (Gupta and Deo, 2022). Before the reactions, the catalysts are reduced at 870 $^oC$ for 2 h to form the active metal sites. The catalytic reactions are performed in a downward-flow quartz tube (packed-bed) reactor, operating in a temperature range of 300–600 $^oC$ under atmospheric pressure (1 atm). The optimal ammonia conversion is observed at a Ni loading of 15 wt. %. Based on this Ni loading, three bimetallic $Ni_3Fe/Al_2O_3$ catalysts are synthesized: (i) one with a total metal loading of 15 wt.%, (ii) another with Ni loading fixed at 15 wt.%, and (iii) a third prepared via sequential impregnation of Fe on $15\,Ni/Al_2O_3$. Among these, the catalyst with a total 15 wt% $Ni_3Fe$ loading showed higher ammonia conversion as compared to other bimetallic and monometallic $15\,Ni/Al_2O_3$ catalysts. The physicochemical properties of the fresh, reduced, and spent catalysts were characterized using various techniques, including X-ray diffraction (XRD), hydrogen-temperature programmed reduction ($H_2$-TPR), $N_2$-physisorption, energy dispersive X-ray spectroscopy (EDX) and transmission electron microscope (TEM), to explain the behavior observed in experiments.

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# Modeling the Stability of Sub-Nanometer Clusters Supported on Amorphous Surfaces via Multiscale Simulations and Machine Learning

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## Abstract

Sub-nanometer metal clusters supported on amorphous oxides are active for several industrial reactions. These catalysts present a distribution of active sites that cannot be precisely characterized using microscopy and spectroscopy techniques. The underlying disorder of the amorphous support further complicates characterization. Furthermore, sub-nanometer clusters form an intractably large configurational space that is not readily sampled using ab initio computational methods, such as density functional theory (DFT). Consequently, the active site distribution and the structure of these catalysts remain poorly understood.

Exploring materials with large configurational spaces over non-equilibrium environments remains an open challenge. In this work we propose the development of an active learning ML algorithm combined with a global-minima finding method to efficiently discover stable metal cluster configurations on amorphous supports. We apply the framework to model amorphous SiO2-supported Pt clusters. Here we present a machine-learned potential (MLP) trained on DFT-energies and forces for Pt/SiO2 clusters. The trained MLP enables fast calculations with DFT-accuracy, significantly reducing the computational cost of exploring the large configurational space of Pt/SiO2. Once developed, our framework will be readily applicable to investigate several different metal-support combinations.

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# Mathematical Modelling of Microbial Biofilms and Swarms

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## Abstract

Bacterial swarming and biofilm formation are collective multicellular phenomena that enable microbial communities to colonize and spread on hydrated surfaces. Understanding bacterial spreading is crucial for infection control, biofilm engineering, industrial pipeline maintenance, and wastewater treatment applications. In this study, we develop a two-phase thin film model to investigate the spreading dynamics of bacterial swarming and biofilm formation, incorporating wetting phenomena. The model accounts for substrate wettability by introducing a disjoining pressure term in the normal stress balance. Our results demonstrate that wettability plays a key role in bacterial spreading dynamics, with increased substrate wettability accelerating the radial expansion of both swarming colonies and biofilms. These results emphasize the critical role of surface properties in microbial motility and provide a more comprehensive theoretical framework for understanding bacterial spreading on hydrated substrates.

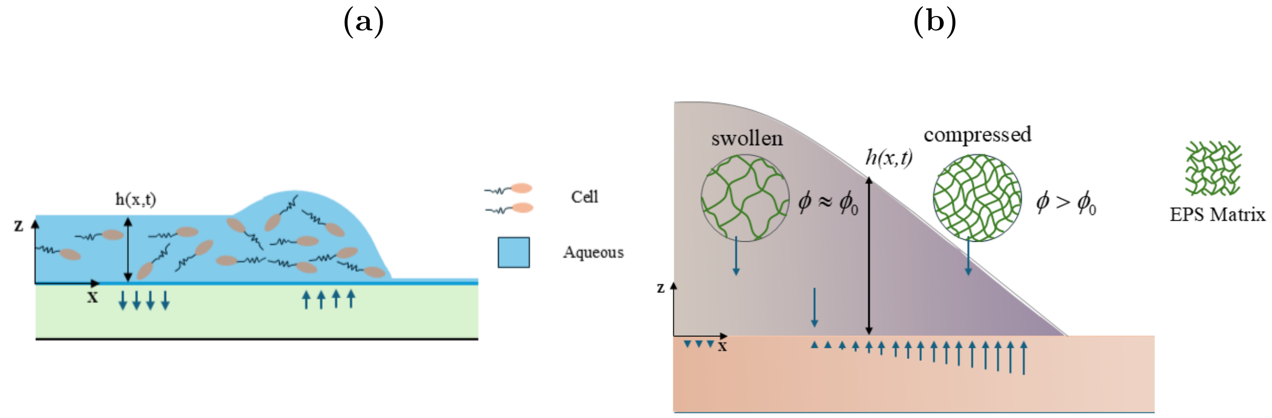

Figure 1: Schematic of $(a)$ bacterial swarm and $(b)$ biofilm on a substrate.

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# Phase-change-driven instabilities in thin film flow over a vertical cylinder

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## Abstract

This study examines the dynamics of a thin liquid film flowing down a vertically heated cylindrical surface under the influence of gravity while accounting for evaporation effects. By employing the lubrication approximation, the governing system is reduced to an evolution equation incorporating key dimensionless parameters, including evaporation number (which characterizes the ratio of convective to evaporative timescales), Thermodynamic parameter ($K$), Marangoni number ($Ma$), and effects of long-range molecular forces ($\Pi$). These parameters critically influence the film's stability, particularly in the presence of both intermolecular interactions and evaporation. To model mass loss at the liquid-gas interface, a one-sided evaporation model is introduced. The film remains sufficiently thin for the continuum approximation to be valid while also allowing long-range molecular forces to play a significant role. For weaker evaporation effects, the film transitions into a time-periodic regime, whereas a steady state is achieved only under strong evaporation and small values of thermodynamic parameter ($K$). Linear stability analysis reveals that evaporation and thermocapillary stress contribute to film destabilization, while long-range molecular forces provide a stabilizing effect. The thermodynamic parameter exhibits non-monotonic behavior, with the highest instability occurring at $K = 1$. Deviations from this value, whether increasing or decreasing, enhance film stability. Furthermore, a comparison between varying mass flux and constant mass flux ($J = 1$) demonstrates that the film exhibits small amplitude oscillations for$J = 1$, thereby promoting film stability.

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# Continuum Modeling of Granular Flow Through Hoppers

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## Abstract

Granular materials are commonly involved in geophysical flows and are widely used in many industries. Discrete Element Method (DEM) simulations are commonly employed to simulate granular flow behavior. Due to the enormous computational cost of large-scale DEM simulations, accurate and efficient continuum simulation of granular materials is highly desirable.

In this work, we perform continuum simulations of the flow behavior of granular materials in a rotating drum. We extend the interFoam solver used for two-phase fluid simulations in OpenFOAM for simulating dense granular flow in the presence of air. The numerical framework involves solving the continuity equation and momentum balance equations for both the granular and air phases. The interFoam solver utilizes the Volume of Fluid (VOF) method, which accounts for the movement and distribution of the interface between the two fluid phases. The granular phase is modeled as a continuum employing the $\mu$-I rheology proposed by Jop et al. (2006), while the fluid phase is simulated as a Newtonian fluid in the laminar regime.

Simulations are performed for both single and multi-orifice hoppers. In single-orifice hoppers, we investigate the influence of orifice size and hopper inclination on granular flow behavior. For multi-orifice hoppers, the effect of orifice eccentricity on flow characteristics is analyzed. A grid dependency test has been performed, with mesh sizes ranging from coarser to finer grids, to ensure that the simulated flow properties remain consistent across varying grid sizes. We were also able to predict key flow properties, including velocity, pressure, inertial number, and flow rate, providing valuable insights into the behavior of granular materials in hoppers.

# $NiBO_3$ (B = Ti, Sn) anchored g-$C_3N_4$-based ternary composite for enhanced photocatalytic hydrogen production via water splitting

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## Abstract

The study deals with the development of a dual-S scheme heterostructure comprising $NiTiO_3$, g-$C_3N_4$ (gCN), and $NiSnO_3$, via a simple ultrasonication-calcination-ultrasonication method. The study includes a detailed physicochemical, optical, and photo-electrochemical characterization of the synthesized material, revealing the efficient photogenerated charge carrier separation and improved charge transport, facilitated by the dual S-scheme heterojunction. The ternary composite harnesses the synergistic effects of dual S-scheme charge transfer and exhibits an outstanding hydrogen evolution rate of 1370 $\mu molg^{-1}h^{-1}$, surpassing the rates of conventional gCN-supported $ABO_3$-type perovskite heterostructures. The material also demonstrates remarkable photostability and recyclability, maintaining high activity after five cycles. The exceptional performance of the $NiTiO_3$-gCN-$NiSnO_3$ composite is attributed to the favorable band alignment and optimal interfacial contact between the components, which facilitate efficient charge transfer and suppress recombination. This study provides valuable insights into the rational construction of the dual S-scheme heterostructures for sustainable hydrogen production and environmental remediation applications.

**Keywords:** hydrogen evolution reaction; perovskite; dual-S scheme heterojunction; photocatalysis; graphitic carbon nitride.

# The Role of Substrate Elasticity on the Physics of Electrowetting

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## Abstract

Electrowetting is a process that alters the wettability of a surface by applying an electric field. As the applied voltage increases, the electric field reduces the macroscopic contact angle, enhancing droplet spreading Dey et al., 2019. Electrowetting on soft dielectric has a wide variety of applications including nanofabrication, high-power energy harvesting, biochemical detection, and several other forms of miniaturized on-chip technologies Kumar, Dhar, and Chakraborty, 2025.

A reduced-order model based on lubrication theory is developed to study the electrowetting of a sessile droplet on a soft dielectric under an applied electric field, considering a pinned electrode configuration. Thin-film evolution equations are obtained for the fluid-fluid interface and fluid-dielectric substrate. The presence of surfactants reduces the wettability of the droplet in the absence of an electric field. In the case of electrowetting over viscoelastic dielectric, an increase in the electric field and surfactant concentration leads to the reduction in contact angle and increase in the contact line radius. By increasing the softness of the dielectric, the extent of electrowetting decreases.

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# Coiled Flow Inverter-Assisted Green Synthesis of $Fe_xO_y$/g-CN Nanoparticles for Sustainable Energy and Environmental Remediation

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## Abstract

Nanoparticles have gained significant attention due to their tunable physicochemical properties, making them invaluable in renewable energy, environmental remediation, and catalysis. However, traditional batch synthesis methods suffer from drawbacks such as poor reproducibility, inefficient mixing, and scalability challenges. Coiled flow inverter (CFI) has emerged as an alternative for continuous flow synthesis, offering precise control over reaction conditions, uniform mixing, and improved reproducibility. In this study, $Fe_xO_y$ doped graphitic carbon nitride ($Fe_xO_y$/g-CN) nanoparticles were synthesized using a CFI reactor, employing green tea extract as a natural reducing and stabilizing agent. This biogenic approach eliminates the need for hazardous chemicals, ensuring an eco-friendly, scalable, and reproducible nanoparticle synthesis method. The CFI-assisted synthesis enables uniform dispersion, good control over Fe-loading in the catalyst, and high-throughput production, overcoming the limitations of conventional batch processes. The synthesized $Fe_xO_y$/g-CN nanoparticles demonstrate excellent potential for green hydrogen evolution via electrocatalysis and continuous photo-biocatalytic denitrification of wastewater. Their superior charge transfer efficiency, catalytic stability, and light absorption properties make them promising candidates for sustainable energy production and environmental remediation. This study underscores the CFI's potential in advancing green nanotechnology, offering a scalable and cost-effective solution for clean energy and water treatment applications.

**Keywords:** Coiled flow inverter; graphitic carbon nitride; electrocatalysis; denitrification; photo-biocatalysis; hydrogen evolution reaction.

# Enhancing ML Accuracy with Domain Adaptation for Small Molecular Datasets

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## Abstract

Advances in high throughput experimental techniques have led to an exponential increase in experimental data, including the synthesis of molecules and their properties. Access to vast amounts of data has enabled the application of machine learning (ML) methods to develop structureproperty relationships and discover new molecules. However, several areas still remain challenging, particularly with expensive and time-consuming experiments, resulting in limited data and making the effective application of ML methods challenging. Domain adaptation, a ML technique where models trained on large datasets are adapted to predict properties of smaller, specialized datasets, offers a promising solution. Structure-property correlations learned from large molecular datasets can be applied to smaller datasets through domain adaptation, improving ML accuracy.

In this work we apply different domain adaptation methods, including TraAdaBoost, TraAdaBoostR2, and Kernel Mean Matching, to transfer knowledge from large structure-property datasets to specialized smaller datasets. As a first application we apply our framework to predict properties of a small dataset of C=O group compounds using correlations learned from a large dataset of pure hydrocarbons (no C=O groups). We apply our framework to predict HOMO-LUMO gap, polarizability, and heat capacity.

Our results demonstrate that domain adaptation improves the accuracy of ML methods for small datasets for various properties. This work paves the way for applying domain adaptation to develop structure-property relationships for scenarios with limited experimental data.

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# Viscoelastic cross-stream migration and the influence of electrokinetics

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## Abstract

The cross stream migration of rigid spheres in both Newtonian and non-Newtonian(viscoelastic) fluid flows has been a subject of extensive research due to its significance in microfluidic applications, industrial processes, and biological transport. For Newtonian fluids, inertial effects play a crucial role in cross-stream migration. In the absence of inertia (Stokes regime), a rigid sphere cannot migrate across streamlines. However, experimental studies confirm lateral migration in pressure-driven flows, leading to the well-known Segre-Silberberg effect. In the case of viscoelastic migration, additional forces arise due to polymeric normal-stress differences. These lateral forces can aid in particle migration even at vanishingly small inertia. In this work, we focus on the latter and examine how viscoelastic lift can be electrokinetically influenced and aim to understand how this modification is fundamentally different from magnetic/gravitational influence.

By incorporating the effects of electrophoresis, we derive an analytical expression for the modified lift force. The results indicate a significant enhancement in migration due to the electrophoretic slip at the particle surface. Finally, we analyze the case of forced migration, where a non-neutrally buoyant particle undergoes sedimentation. The buoyancy-induced lag or lead velocity alters the disturbance flow field, affecting the migration dynamics. Particle trajectory plots illustrate the impact of various factors on lateral migration. The study provides insights into the complex interplay of inertia, elasticity, and external forces in particle migration, offering potential applications in microfluidics, particle sorting, and biomedical engineering.

***Keywords***: Inertial migration, viscoelastic migration, Electrophoresis, Gravitational Migration.

# Kinematics of minimal model microswimmers

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## Abstract

The simplest three-sphere swimmer by Najafi and Golestanian is made from three spheres that are connected by two arms which change their lengths periodically in non-reciprocal manner. Here we study a variation of the model in which one arm is replaced by an elastic filament while the other is periodically actuated. We show that the competition between the hydrodynamic drag force and the elastic restoring force produces a phase difference in the response of the passive elastic spring arm with respect to the active arm. This leads to non-reciprocal shape changes and self-propulsion. We study the qualitative properties of the solutions,compute analytically their leading order approximation and compare them with numerical solutions. We also formulate some optimisation problems,aimed at finding the maximizing performance, for various performance measures. This model system could be used in constructing robotic microswimmers.

**Keywords:** non-reciprocal,Elastic restoring force,Hydrodynamic drag force,Microswimmer.

# Sugarcane based sustainable electrodes for the detection of arsenic from rice

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## Abstract

Arsenic, a highly toxic pollutant, poses a significant threat to human and animal health. It infiltrates the food chain by leaching from contaminated soil and groundwater. Hence, there is a need for affordable, real-time systems to measure arsenic levels in food samples. In this work, a gold nanodot-modified sensor was developed using a sustainable sensing platform, SugarcaneSens, to detect arsenic from rice samples. The sensitivity of the sensor was evaluated by anodic stripping differential pulse voltammetry (ASDPV), and a working range of 2 ppb to 1000 ppb with a limit of detection (LOD) of 1 ppb was observed. Two linear response ranges between 2 ppb to 100 ppb and 100 ppb to 1000 ppb were observed with a sensitivity of 0.143 $\mu Appb^{-1}$ cm$^{-2}$ and 0.024 $\mu Appb^{-1}$ cm$^{-2}$ respectively. This sensor exhibited good reproducibility and stability, making it a promising alternative for the detection of arsenic in rice and other food products.

(Gokhale, Dushing, and Panda, 2025).

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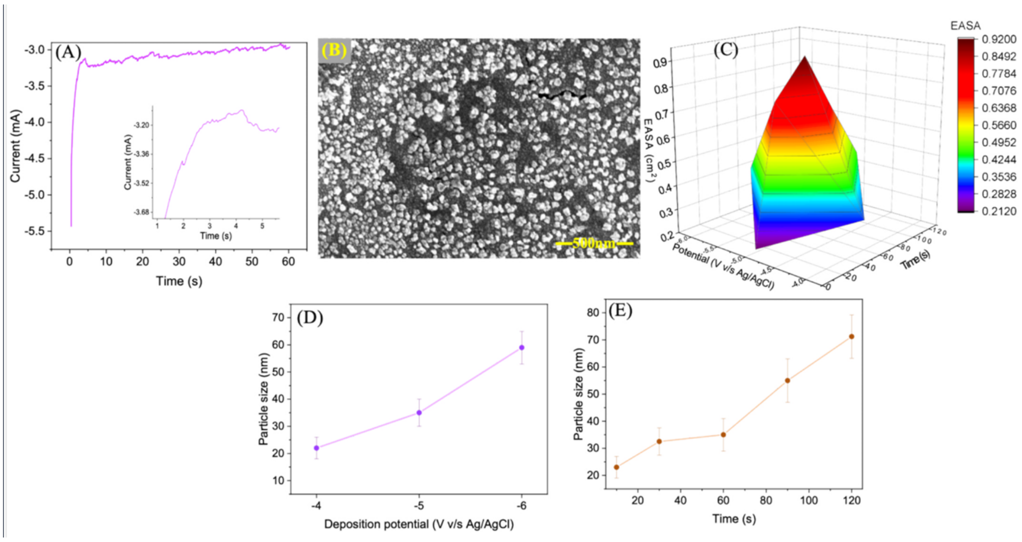

Figure 1: (A) Chronoamperometric profile of deposition at -5V, 60 s in a bath of 1 mM HAuCl4 +10 mM NH4Br (magnified graph in the inset), (B) SEM image of the electrodeposited gold nanodots, (C) 3D contour plot of gold nanodot optimization showing the effect of potential and deposition time on the EASA (D) mean particle size of gold nanodots for various deposition potentials (at t = 60 s) and (E) mean particle size of gold nanodots for various deposition times (at V = -5 V).

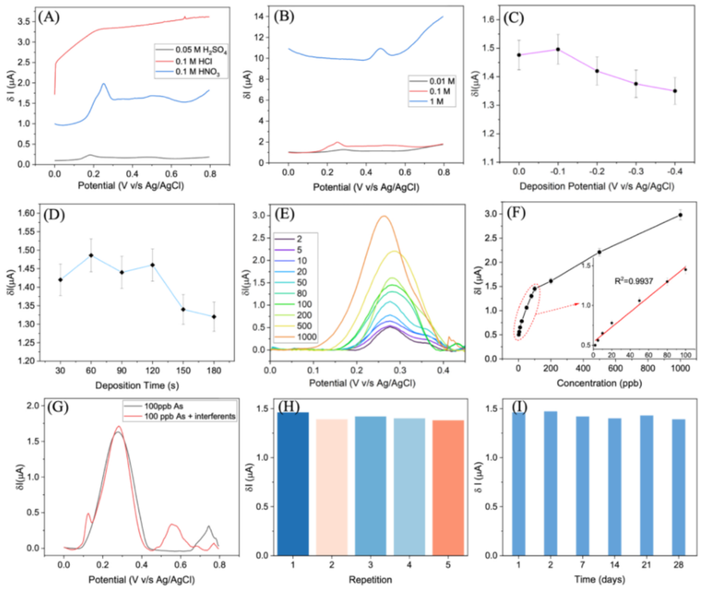

Figure 2: (A) ASDPV response of 10 ppb As(V) in different electrolytes, (B) ASDPV response of 10 ppb As(V) in different concentrations of HNO3 10 ppb As (V) in 0.1 M HNO3 at varied deposition potential, (D) ASDPV response of 10 ppb As (V) in 0.1 M HNO3, (C) ASDPV response of at varied deposition time, (E) ASDPV response of various concentrations of arsenic in 0.1 M HNO3, (F) corresponding calibration plot, (G) ASDPV response for 100 ppb As with and without interferents, (H) reusability test and (I) time stability using the parameters mentioned in materials and methods section.

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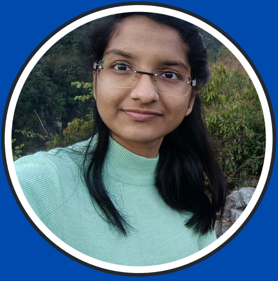

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