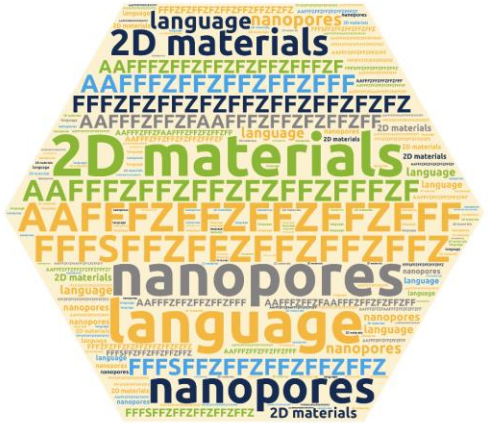
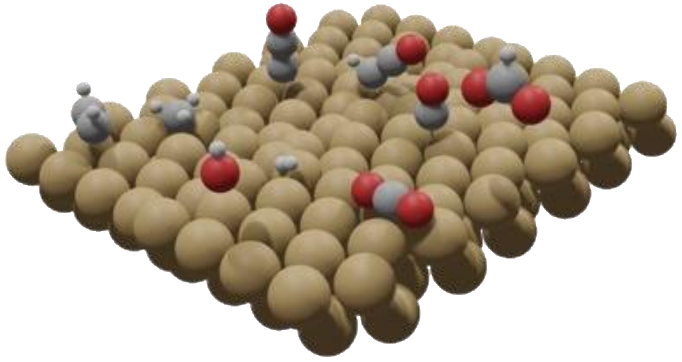
Automated and Accelerated Materials Design Aligned with India's National Priorities





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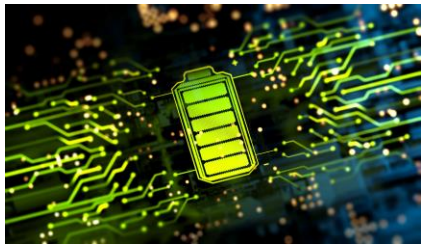
Formulating a National Research Roadmap for Accelerated Materials Design, ICTS
Session I: Perspectives and National Priorities 1
August 31-September 1, 2026

Outline for this talk

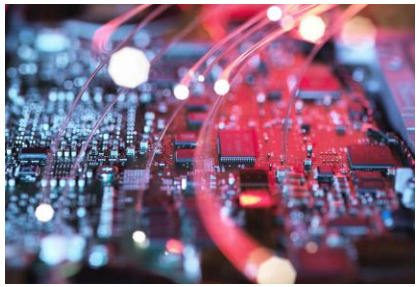
Motivation

Why accelerated materials design, and India's requirement of a national roadmap



Materials design use cases

Examples from my group: catalysis, 2D magnets, 2D membranes, in areas relevant to national missions



Current status of materials discovery

AI/ML for materials efforts in India; where global academia and industry are

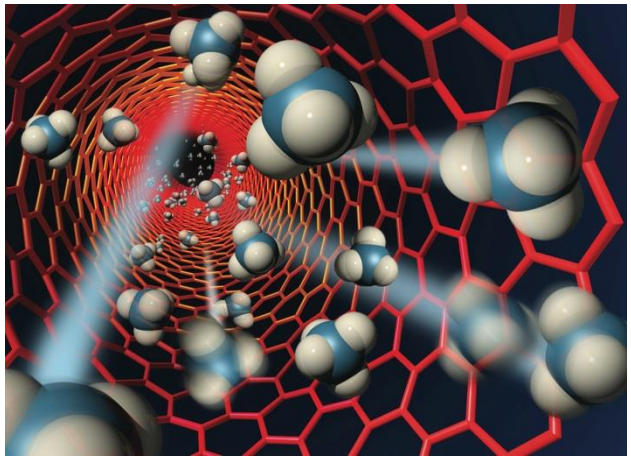
Where India stands

Strengths, gaps, and questions towards Discussion 1.1

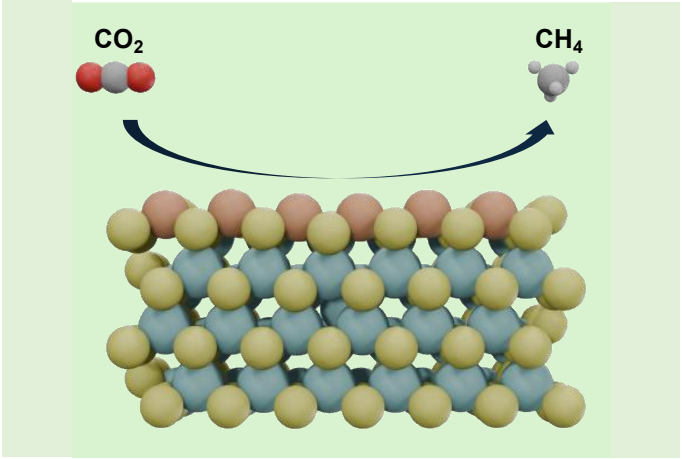
Example project

AIM-ACCELMAT: an example of this type of roadmap under ANRF's AI for Science and Engineering Mission

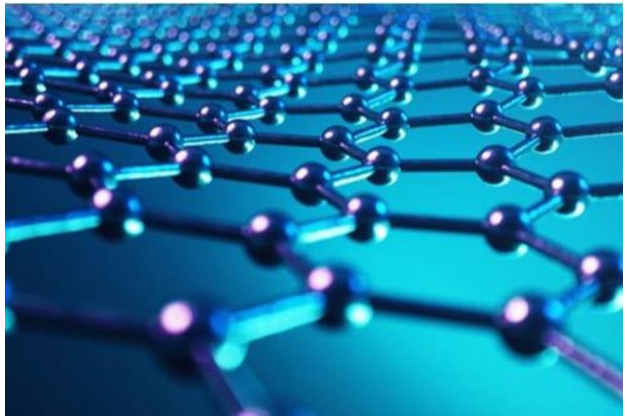
Building today's technologies requires us to understand atoms and electrons



CO_2 capture and desalination



Catalysis and energy conversion



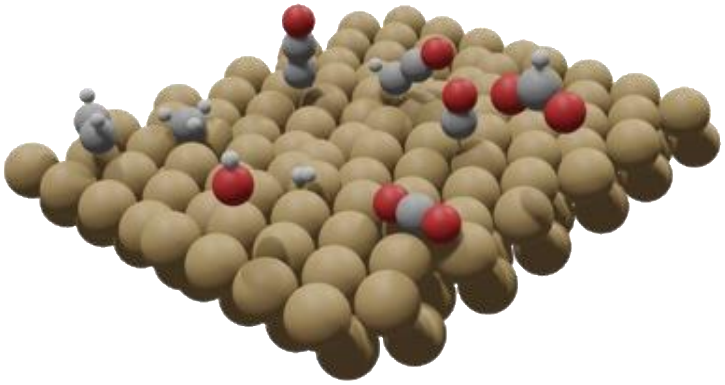
Nanomaterial synthesis

Trial-and-error based choice of materials and operating conditions for various applications

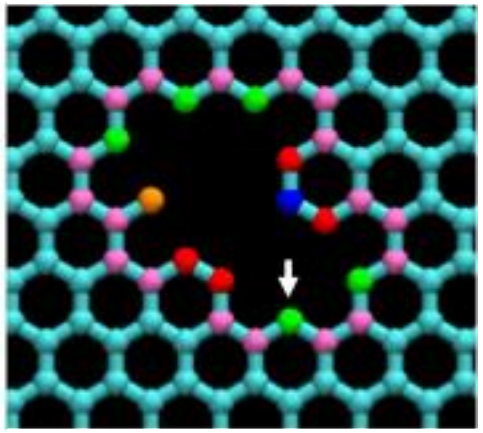
Optimal materials and process parameters using atomic-level simulations and AI/ML

Images adapted from: cdiglobal.com, investingnews.com

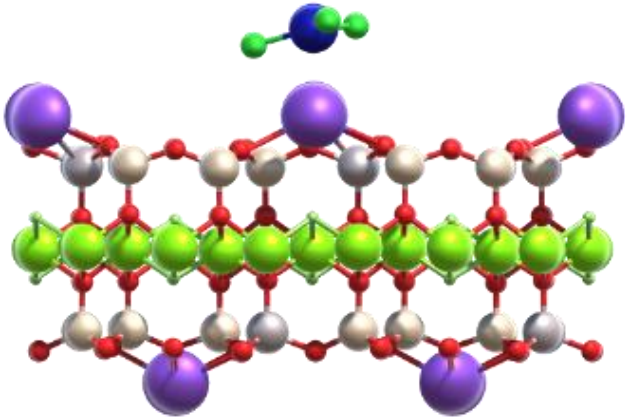
In silico research areas of interest in our group



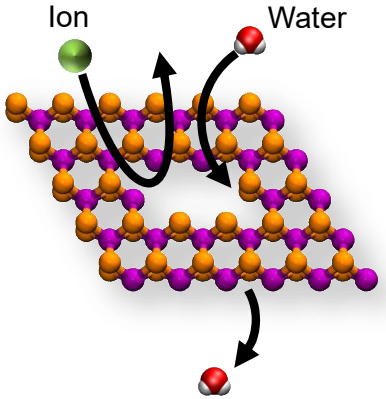
Modeling of catalytic and electrochemical processes

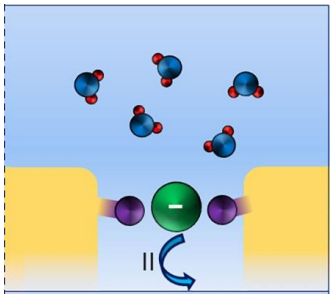


Formation of nanopores and structure-performance relations in nanoporous membranes



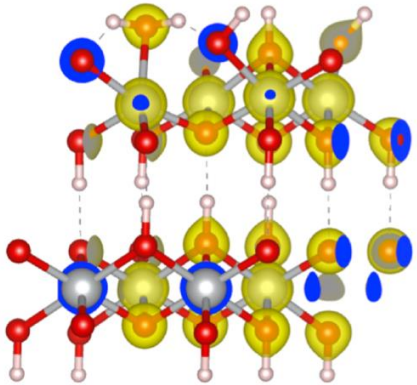
Understanding synthesis of 2D materials





Nanoscale molecular and ionic transport phenomena

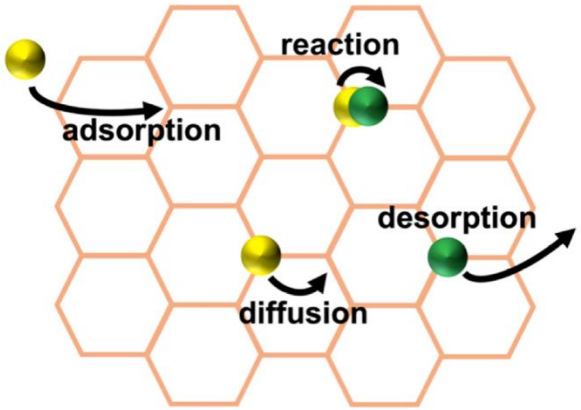
Combined classical and quantum mechanical simulation for nanoscale thermodynamics and kinetics



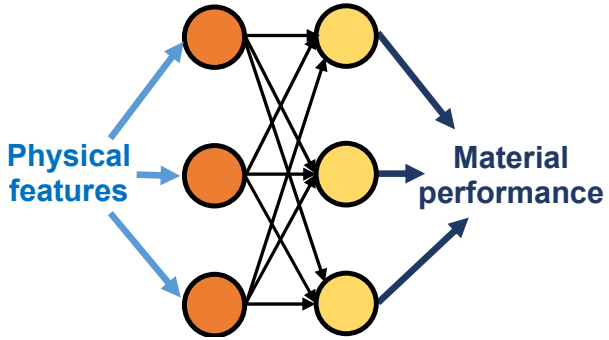
Reaction rate and equilibrium constants

Atomic forces and potential energies

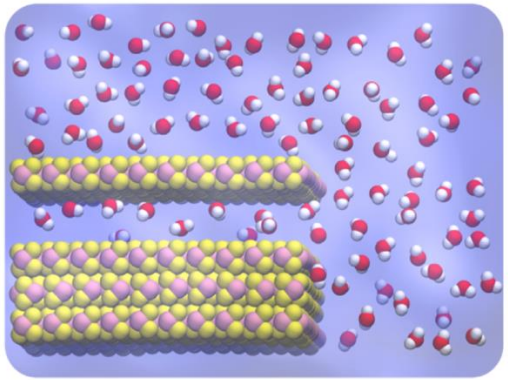
Density functional theory (*DFT*)
reaction free energies and barriers



Kinetic Monte Carlo (*KMC*)
nanopore formation
and material synthesis



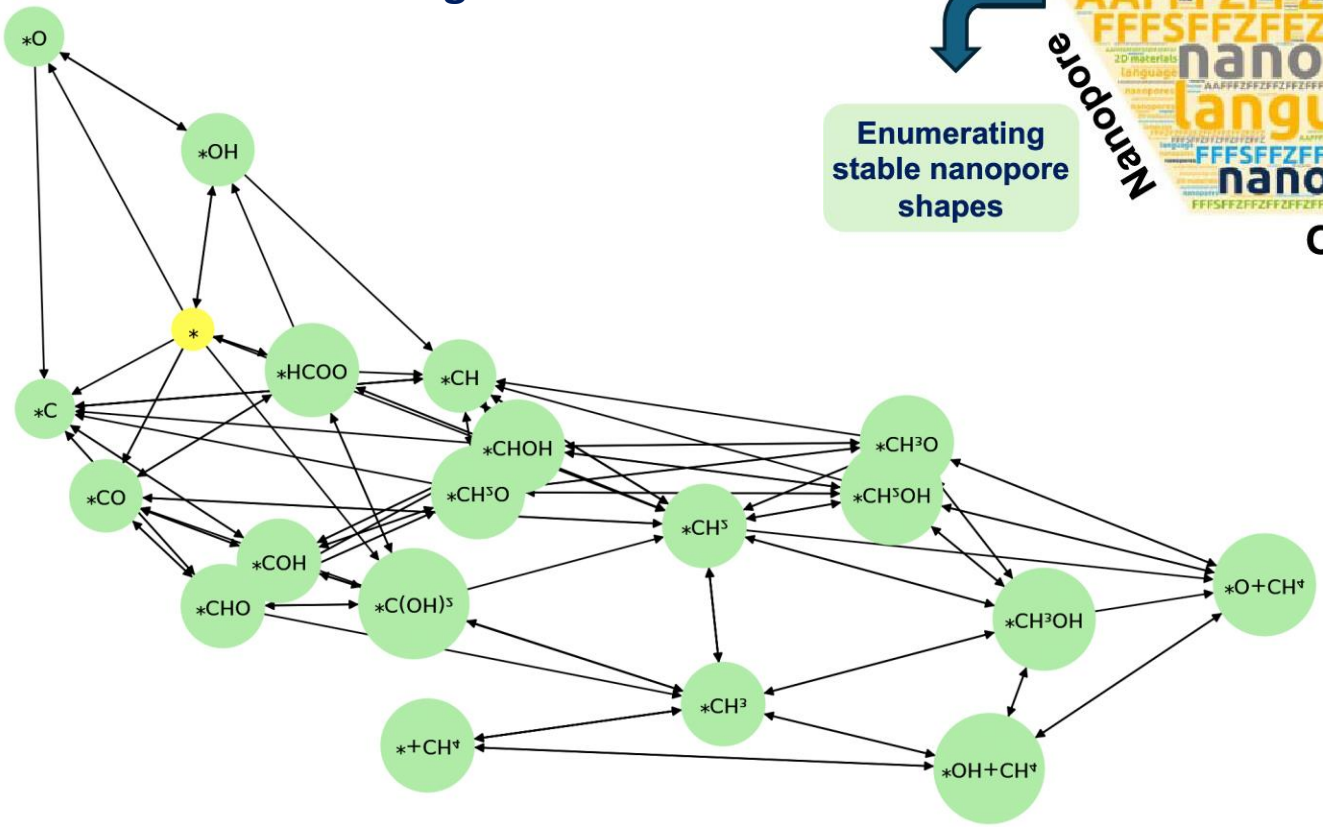
Machine learning (*ML*)
prediction and discovery
of nanomaterials for energy/water



Molecular dynamics (*MD*)
nanoscale transport
phenomena

Materials and mechanism discovery in nanomaterials via AI/ML strategies

What is the best membrane structure for a required separation; can we create membrane digital twins?



What is the most-probable mechanism and the resultant kinetics & thermodynamics of CO_2 hydrogenation?

Sharma, Govind Rajan, et al. *J. Am. Chem. Soc.* **2024**, 146, 30126; White et al., *Chem. Rev.* **2015**, 115, 12888

From the global perspective to India

Global: the self-driving lab wave

- AI proposes candidate materials in silico (generative + screening models)
- Robots synthesize and characterize them, 24/7, without waiting on a human
- Berkeley's A-Lab and Toronto's Acceleration Consortium demonstrate discovery cycles shortened by orders-of-magnitude
- By 2026, lab demos are moving toward real infrastructure

India: a mission-mode manufacturing push

- About ₹2 lakh crore announced across critical minerals, magnets, green hydrogen, batteries, and semiconductors
- Each of these missions involves materials design problems (cost, supply chain, efficiency, etc.)
- Timelines are ambitious (5-10 years), but existing discovery cycles are slow to match them

Materials priorities across India's strategic missions

Several national priority areas require materials design and discovery capabilities

Catalysts

National Green Hydrogen Mission

₹19,744 crore · ₹400 cr R&D

Import-substitution for industrial & green-hydrogen catalysts

Carbon capture, utilization, & storage

CCUS Program, Budget 2026-27

₹20,000 cr · 5 years

Capture materials, membranes & sorbents for power, steel, cement & chemical industries

Semiconductors

India Semiconductor Mission 2.0

₹1,27,500 cr

12 units approved, 3 in production; targets fab materials & gases too

Battery materials

ACC battery Production-Linked Incentive

₹18,100 cr · 50 GWh goal

Only ~1.4 GWh commissioned as of Oct. 2025

Sources: Ministry of Mines (National Critical Mineral Mission); PMO (Rare-Earth Permanent Magnet); Ministry of Heavy Industries & IEEFA (National Program on Advanced Chemistry Cell PLI); National Semiconductor Mission 2.0

Materials priorities across India's strategic missions

Several national priority areas require materials design and discovery capabilities

Critical minerals

National Critical Mineral Mission

₹34,300 cr · FY25-31

30 minerals identified; 1,200 exploration projects planned

RE permanent magnets

REPM Manufacturing Scheme

₹7,280 cr

6,000 MTPA sintered rare-earth magnet capacity targeted

Nuclear materials

Nuclear Energy Mission

₹20,000 cr for small modular reactor R&D

alloys, reactor-vessel alloys, Zirconiumradiation-resistant structural materials

Advanced structural alloys

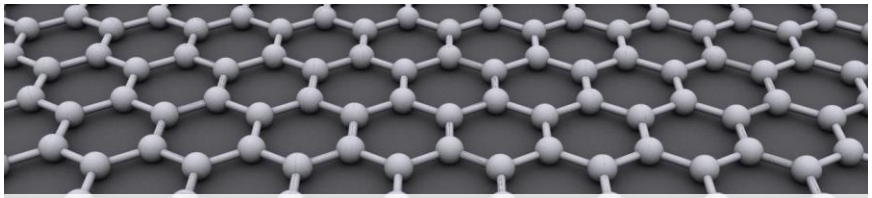
PLI Scheme for Specialty Steel

₹6,322 cr

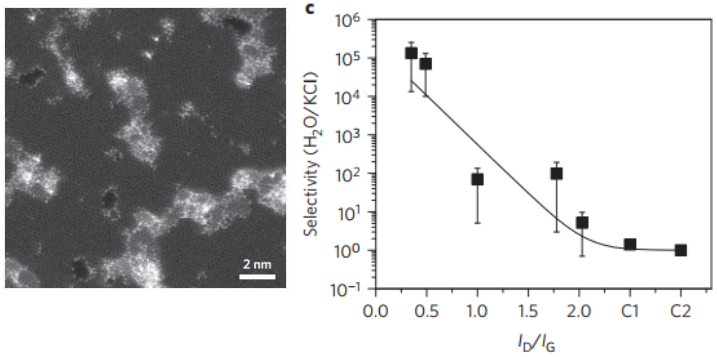
Defence, aerospace, energy & automotive sectors

Sources: Ministry of Mines (National Critical Mineral Mission); PMO (Rare-Earth Permanent Magnet); Ministry of Heavy Industries & IEEFA (National Program on Advanced Chemistry Cell PLI); National Semiconductor Mission 2.0

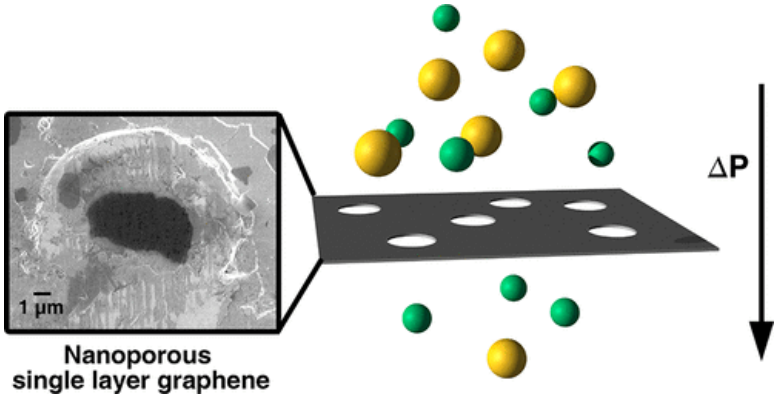
2D materials: the thinnest possible membranes



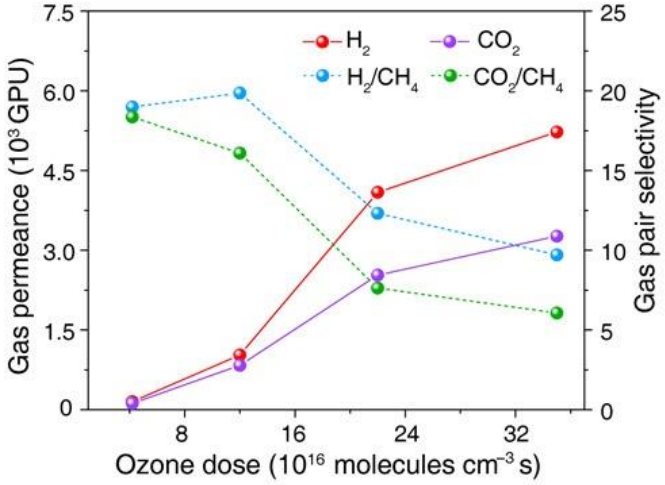
Pristine 2D materials including graphene (a single layer of sp^2 carbon) are impermeable to the smallest molecules, but nanopores in them can enable…



Efficient and high rejection desalination
Surwade et al., *Nat. Nano*. **2015**



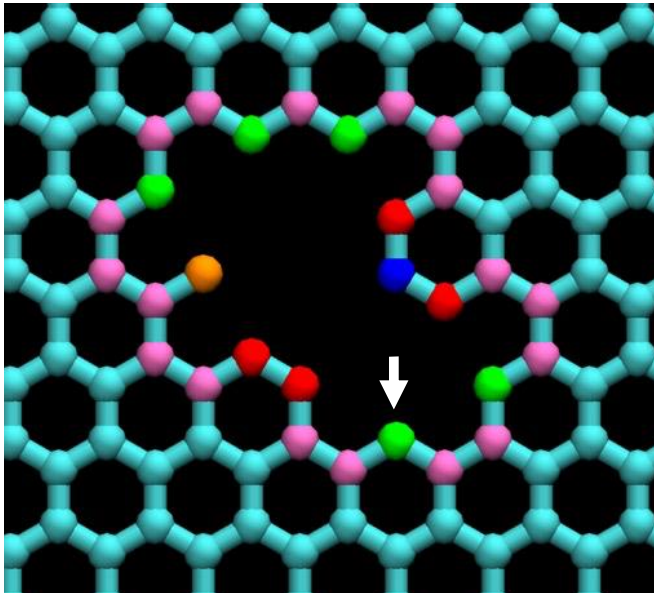
Beyond Knudsen gas-separation membranes
Yuan, Blankschtein, Strano, et al., *Nano Lett.* **2018**



CO_2- and CH_4-sieving nanopores
Huang et al., *Sci. Adv.* **2021**

A language for nanopores based on atom types

Edge atom type	Character
Fully bonded	F
Zigzag	Z
Armchair	A
Corner	C
Singly bonded	S



ZFFZFFFACAFFFZFZFFZFFFSFFAAFF

"STring Representation Of Nanopore Geometry (STRONG)" enables

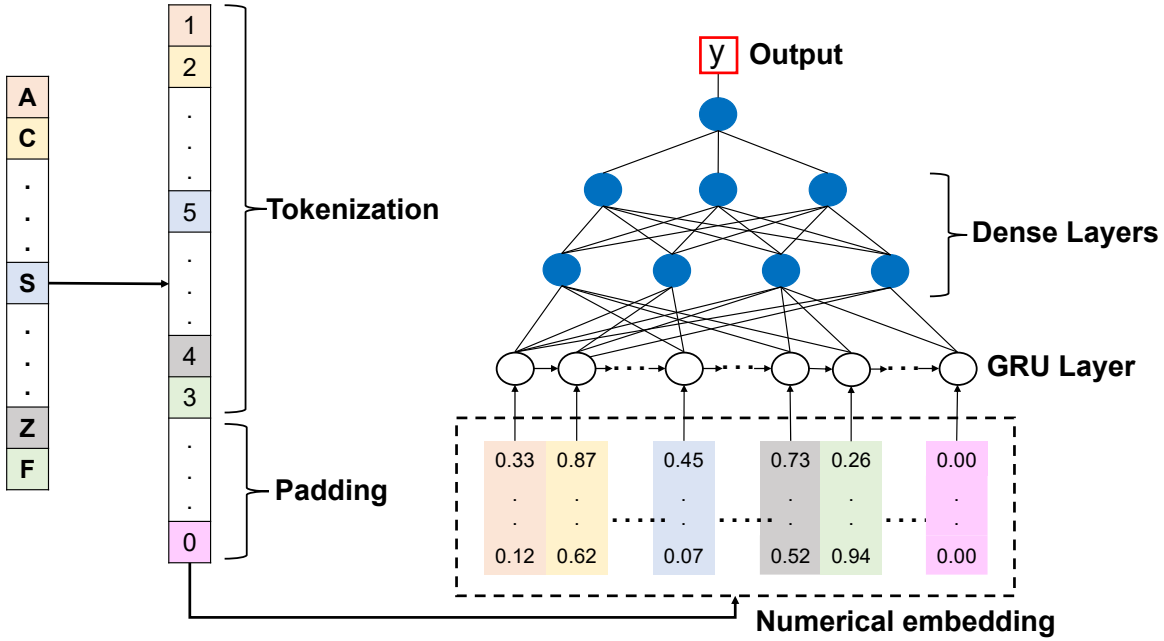
Rapid comparison of nanopore topologies

Enumeration of unique functionalized configurations

Structure-property relationships via neural networks

Sharma, **Govind Rajan**, et al. *JACS* **2024**, 146, 44, 30126

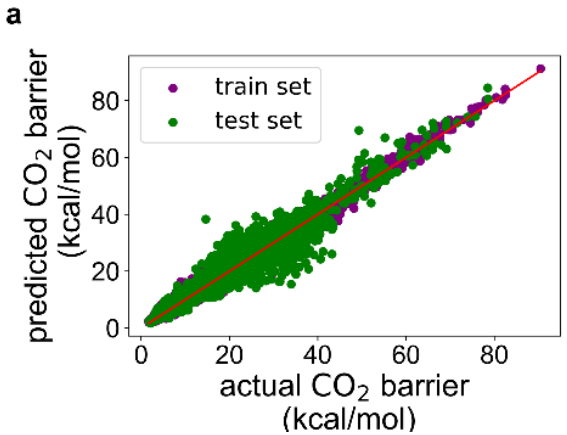
Designing nanopores for CO_2 capture via ML

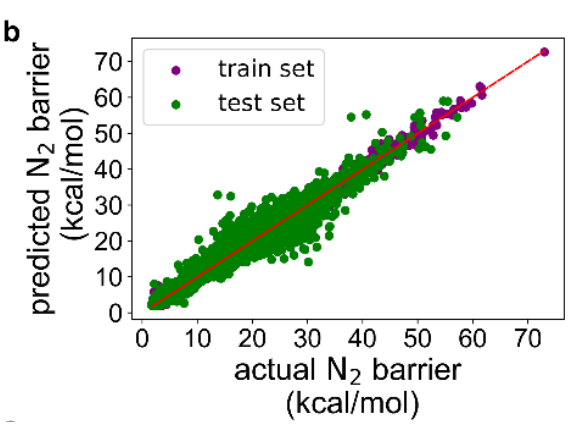


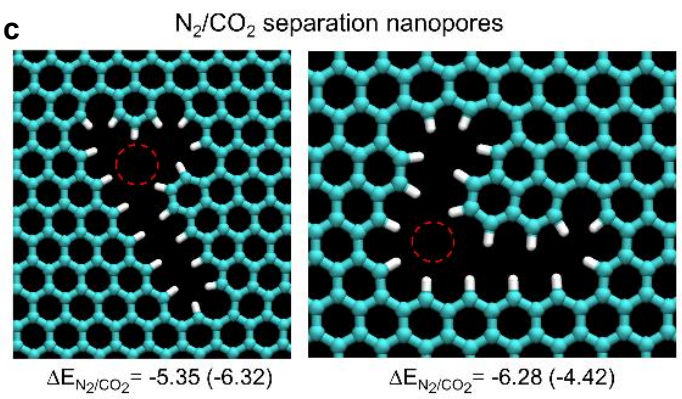
Metric	CO_2 barrier prediction	
	Training set (five folds)	Test set
R^2	0.98	0.95
MAE (kcal/mol)	0.95	1.52

Metric	N_2 barrier prediction	
	Training set (five folds)	Test set
R^2	0.99	0.96
MAE (kcal/mol)	0.65	1.18

Use of recurrent neural networks with a gated recurrent unit (GRU) enables prediction of nanopore properties directly from strings





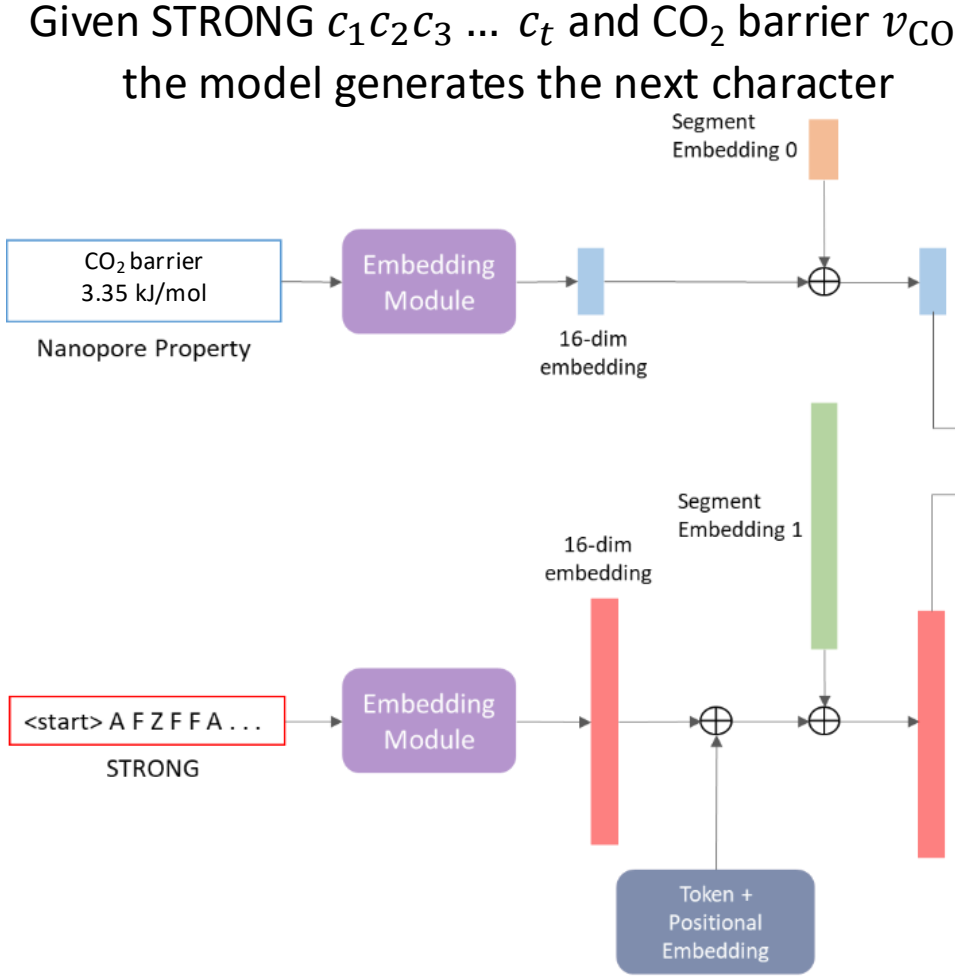


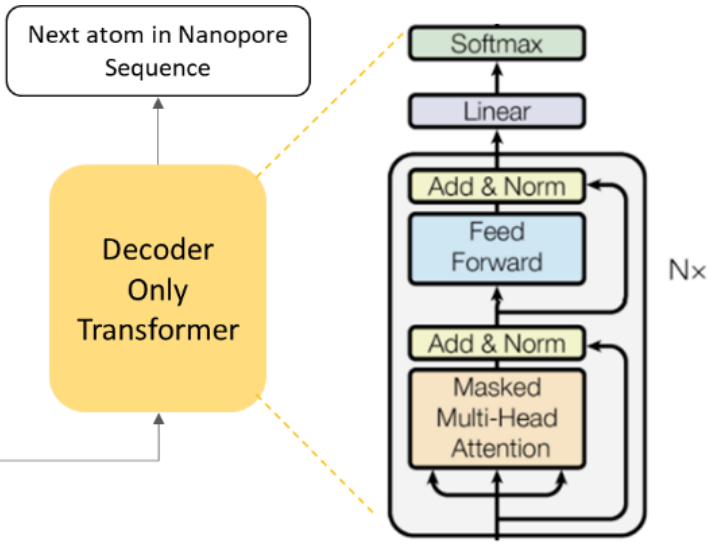
Sharma, **Govind Rajan**, et al. *JACS* **2024**, 146, 44, 30126

From screening 180k stable pores

Inverse design of nanopores via transformer-based generative AI model

Given STRONG $c_1c_2c_3 \ldots c_t$ and CO_2 barrier v_{CO_2}, the model generates the next character





$$\text{Attention}(\mathbf{Q},\mathbf{K},\mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d_k}}\right)\mathbf{V}$$

$\mathbf{Q}$uery, $\mathbf{K}$ey, $\mathbf{V}$alue

Categorical cross-entropy loss

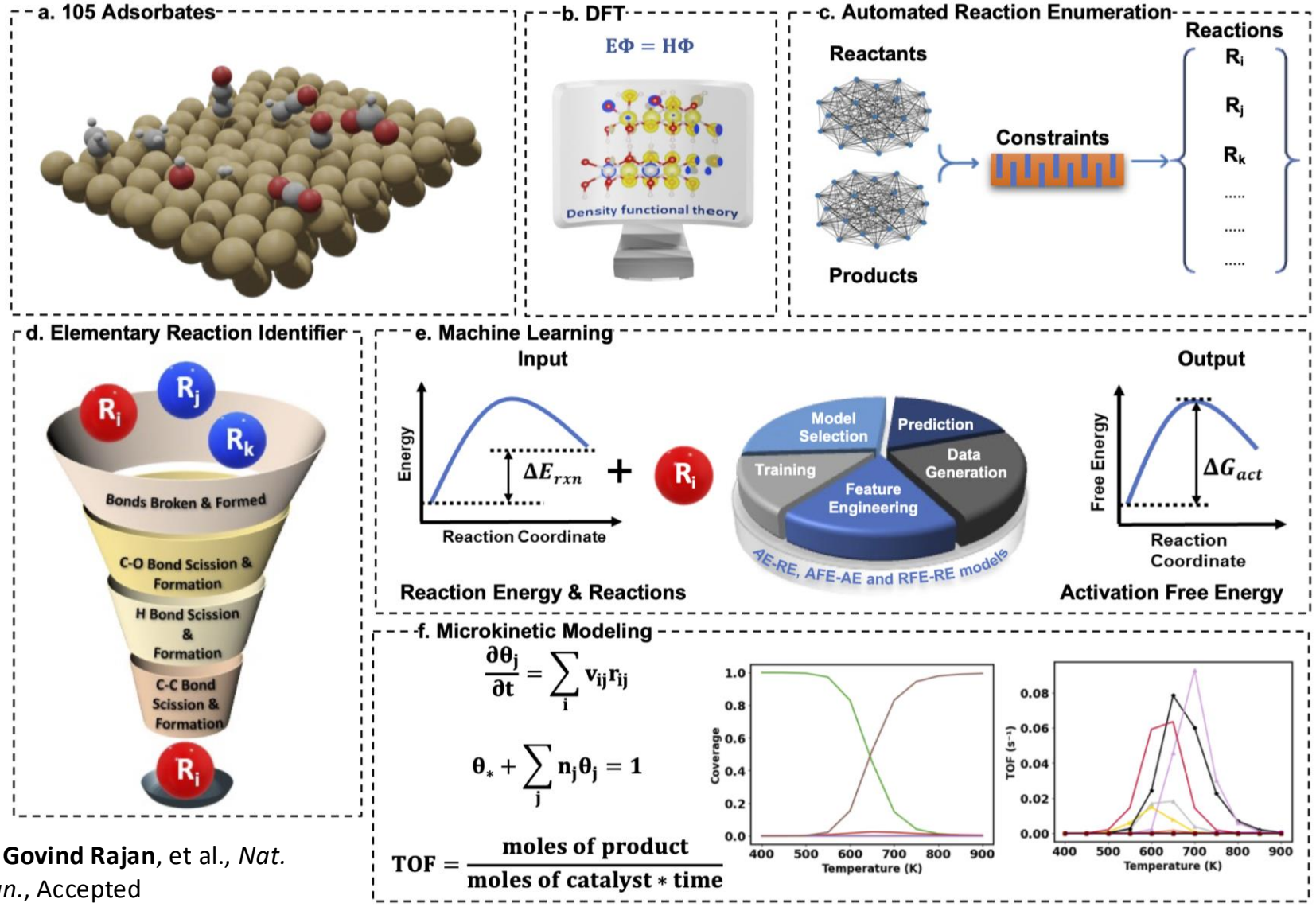
$$L = -\sum_{t=1}^{T} \sum_{i=1}^{|V|} y_t(i) \log P_t(i)$$

T: sequence length, $|V|$: vocabulary size, $y_t(i)$: boolean for character i at timestep t, $P_t(i)$: predicted probability of character i at timestep t

Venkatakrishnan, Lavhekar, and Govind Rajan. In preparation.

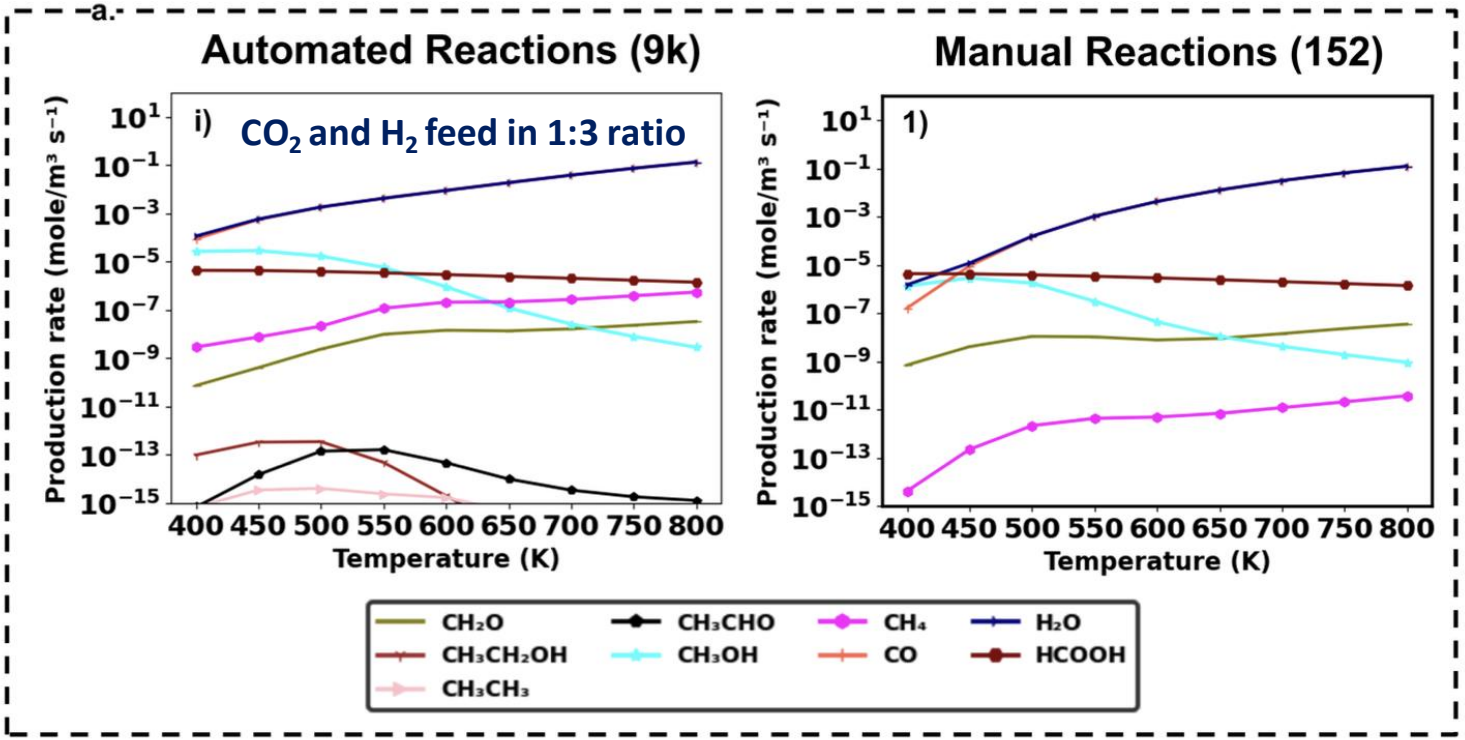
Modeling complex thermocatalytic reaction networks

Experimental studies show CO_2 hydrogenation to methanol on copper; but simulations are not able to predict this to the correct extent. Can we address this?



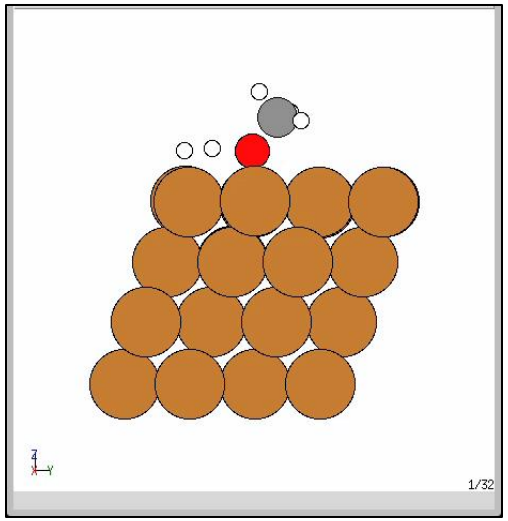
Verma, **Govind Rajan**, et al., *Nat. Commun.*, Accepted

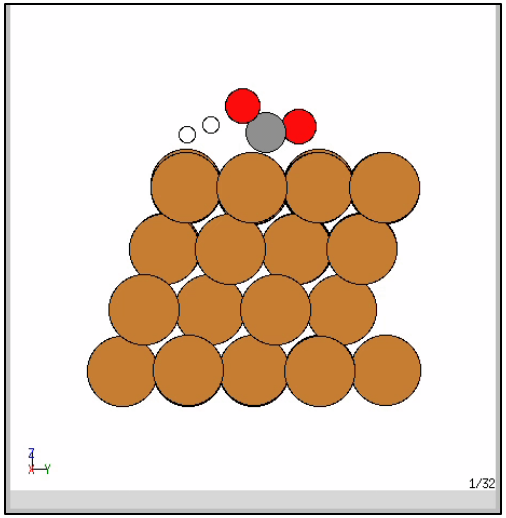
Automated microkinetic modeling with 9k reactions predicts 30-times higher methanol production



Qualitatively agrees with experiment: CO formed more than methanol; formic acid/formate detected via in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS)

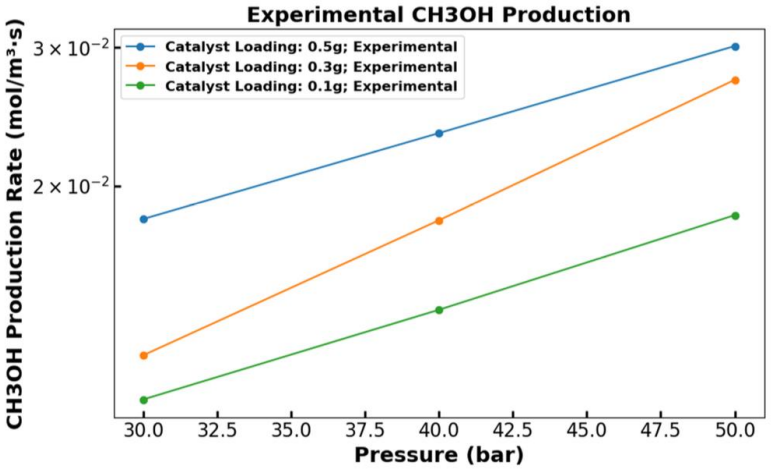
Possibility of direct molecular hydrogenation of intermediates confirmed via DFT

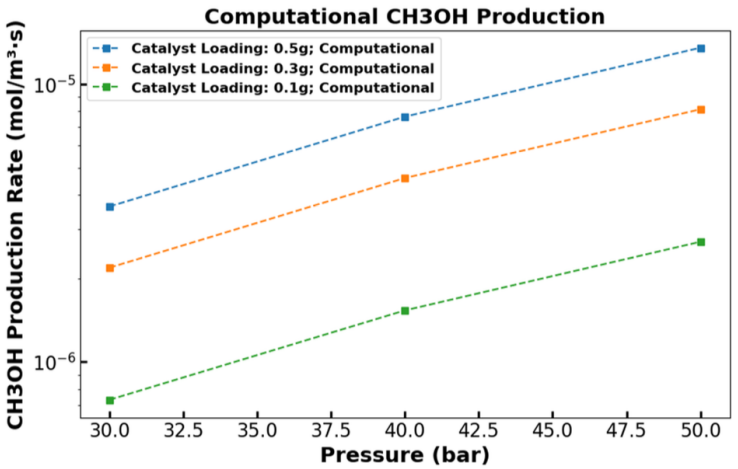




DFT calculations confirm possibility of direct hydrogenation via molecular H_2

Reaction	ML G_{act} (eV)	DFT G_{act} (eV)
$CO_2^* + H_2^* \rightleftharpoons COOH^* + H^*$	0.75	0.61
$CO_2^* + H_2^* \rightleftharpoons HCOO^* + H^*$	0.35	0.18
$HCOOH^* + H_2 \rightleftharpoons H_2COOH^*$	0.48	0.54
$CH_3O^* + H_2 \rightleftharpoons CH_3OH^* + H^*$	0.44	0.44



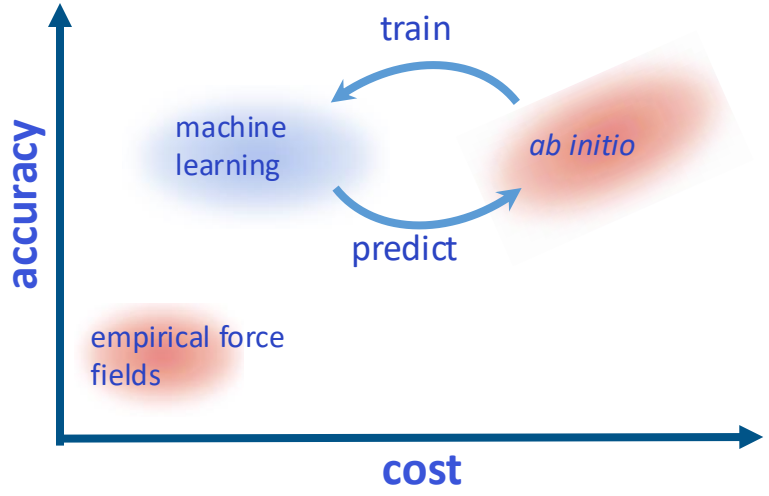


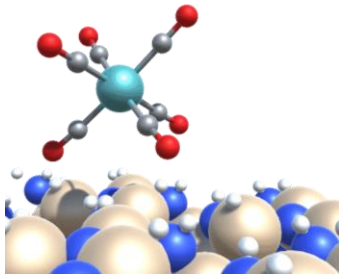
Experimental methanol selectivity of around 10% is close to predictions as well

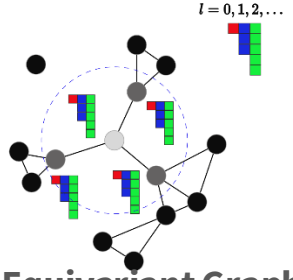
Verma, **Govind Rajan**, et al., *Nat. Commun.*, Accepted

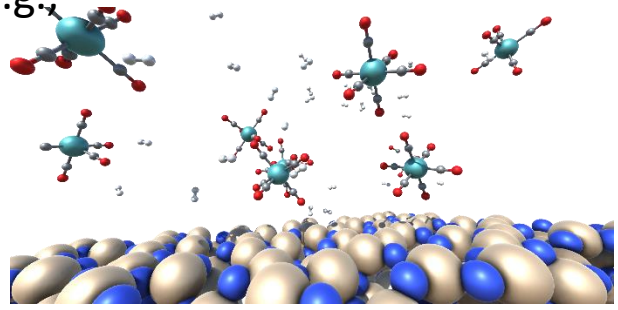
Accelerating nanomaterial synthesis modeling with machine learning interatomic potentials (MLIPs)

- **Ab initio molecular** simulations are **computationally expensive** and limited to **small systems** and **short timescales**
- Need **faster** alternatives **without sacrificing accuracy**
- **Equivariant graph neural networks (GNNs)** trained on DFT data, such as multi-atomic cluster expansion (MACE)[1], capture complex interatomic interactions approaching **DFT-like accuracy**
- State-of-the art **foundation models** trained on millions of datapoints are publicly available (e.g., **MACE-OMAT-0**, **MACE-MPA-0**).



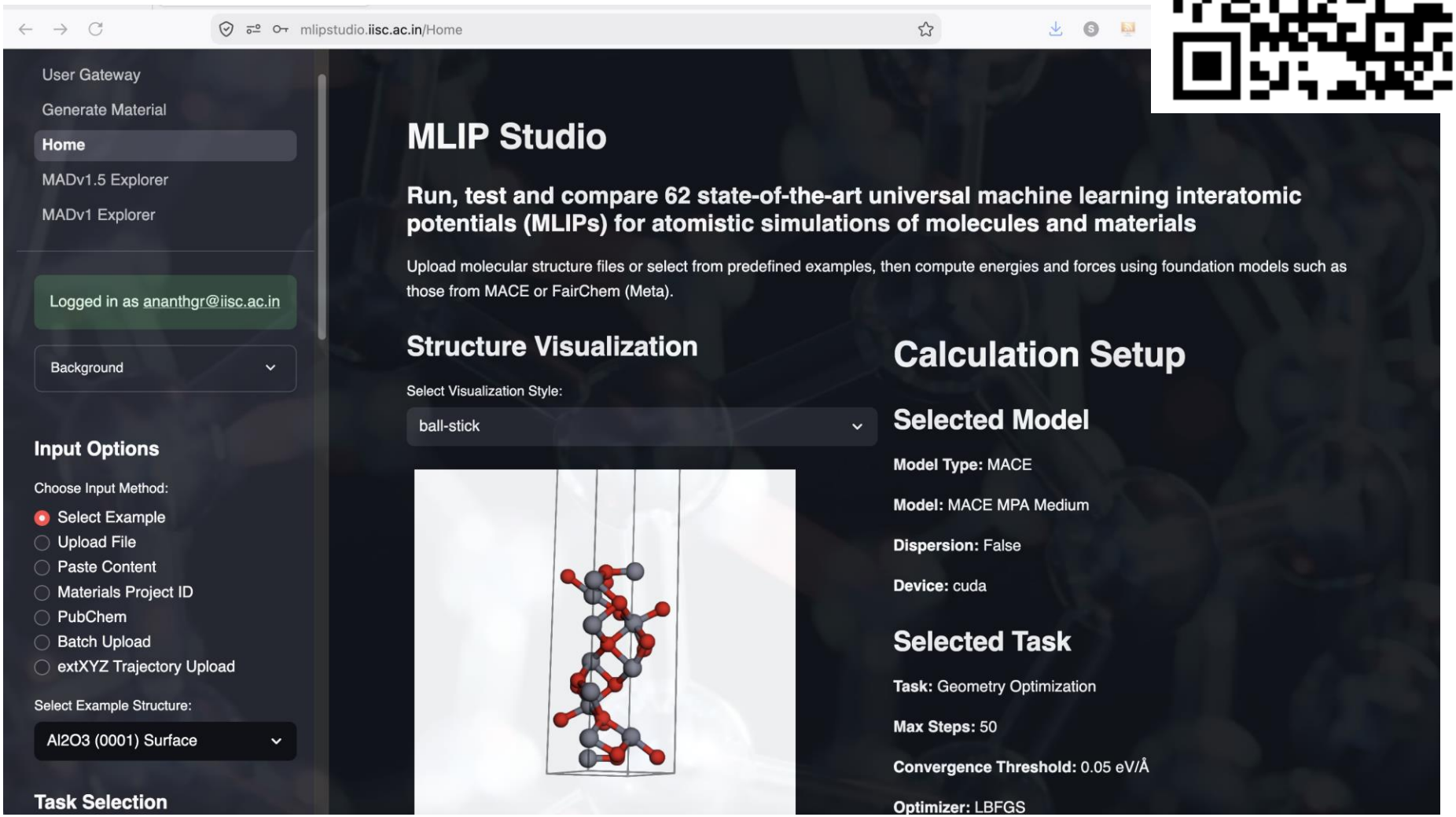






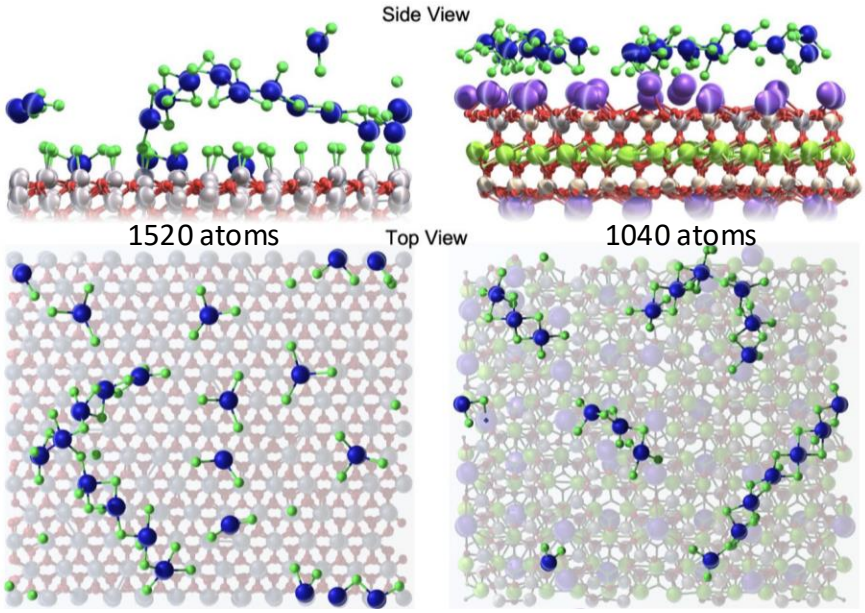
[1]Batatia *et al.*, *NeurIPS* **2022**

MLIP Studio: interactive benchmarking and atomistic simulations using MLIPs



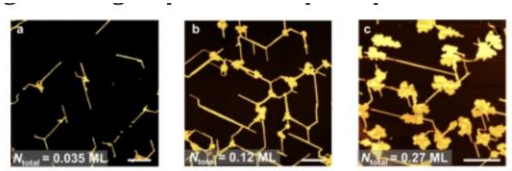
Sharma, Punnathanam, and **Govind Rajan**. *arXiv:2607.07606v1 [cond-mat.mtrl-sci]*

ML molecular dynamics simulations provide insights into deposition of 2D magnetic material $CrCl_3$



- **$CrCl_3$ molecules** on **sapphire do not move** from their **initial positions**
- **Cl** atoms **detach** from $CrCl_3$ on **sapphire**
- Some **$CrCl_3$** molecules are **very close** to the **sapphire** substrate, while some are **farther**
- Almost **all $CrCl_3$** molecules **form chains** on **F-mica**
- **All $CrCl_3$** molecules are at a **similar distance** from the **F-mica** substrate

MLMD details:
NVT ensemble at 800K
Time: 40 ps with a timestep of 0.5 fs
MLIP: MACE OMAT-0



*Lu et al, **Nat. Commun.** 14, 2465 (2023)*

Kumar, Sharma, Punnathanam, **Govind Rajan**, Singh, et al., *Adv. Mater.* **2026**, 38, 34, e14405

MLIP simulations powered by ASE

AI/ML capabilities emerging in Indian materials research

Theme	Breadth of work*
ML-based property prediction models	Band gaps/edges; magnetic, mechanical, and thermodynamic properties; transfer-learning approaches
Applications/assessment of MLIPs	Batteries, aqueous electrolytes, nanoparticle nucleation, 2D materials synthesis, benchmarking strategies,
Materials design	Catalyst/nanopore discovery, inverse design of inorganic materials, reaction-outcome prediction
Knowledge extraction and experimental automation	NLP tools for domain-specific information extraction, stress-testing LLMs and vision LLMs, automation of AFM

***Selected examples; the list is not exhaustive**

Prasenjit Sen, Raghavendra Rajagopalan, Ananth Govind Rajan, and Prasenjit Ghosh, In preparation.

Some overseas autonomous science initiatives: academia

A-Lab, UC Berkeley / LBNL

Originally reported 41 of 58 target compounds synthesized across 17 days of continuous, unattended operation. A 2026 correction revised this to 36 of 57; subsequent re-analysis has raised deeper questions about phase identification and novelty.

Szymanski et al., Nature 624, 86-91 (2023); Palgrave, Schoop, et al. critique PRX Energy, 3, 011002 (2024)

Coscientist, Carnegie Mellon University

An LLM-driven agent that planned and executed real cross-coupling reactions using robotic APIs, with no human decision-making in the experimental loop.

Boiko, MacKnight, Kline & Gomes, Nature 624, 570-578 (2023)

Acceleration Consortium, U of Toronto

A $200M CFREF grant (~$500M with partners) is building large-scale self-driving-lab infrastructure to compress materials innovation from ~20 years/$100M toward ~1 year/$1M. The consortium has also demonstrated AI-driven design of a potential cancer-drug candidate in 30 days.

University of Toronto news release (2023); acceleration.utoronto.ca

Some overseas automated materials discovery initiatives: industry

GNoME, Google DeepMind

2.2 million candidate crystal structures predicted; 380,000 flagged stable and released into the Materials Project. 736 had been independently synthesized by outside labs.

Merchant et al., Nature 624, 80-85 (2023); Materials Project

Azure Quantum Elements, Microsoft + PNNL

Screened 32.6 million candidate materials; synthesized a solid electrolyte using ~70% less lithium; start to working prototype in under 9 months.

Microsoft Azure Quantum blog (Jan 2024)

Toyota Research Institute (AMDD)

$36M committed over 4 years to university partnerships (MIT, Johns Hopkins and others) for AI-accelerated battery and materials workflows and a new Johns Hopkins tie-up was announced this month.

Toyota Research Institute; Johns Hopkins Hub (Aug 2026)

The path forward: Indian perspective

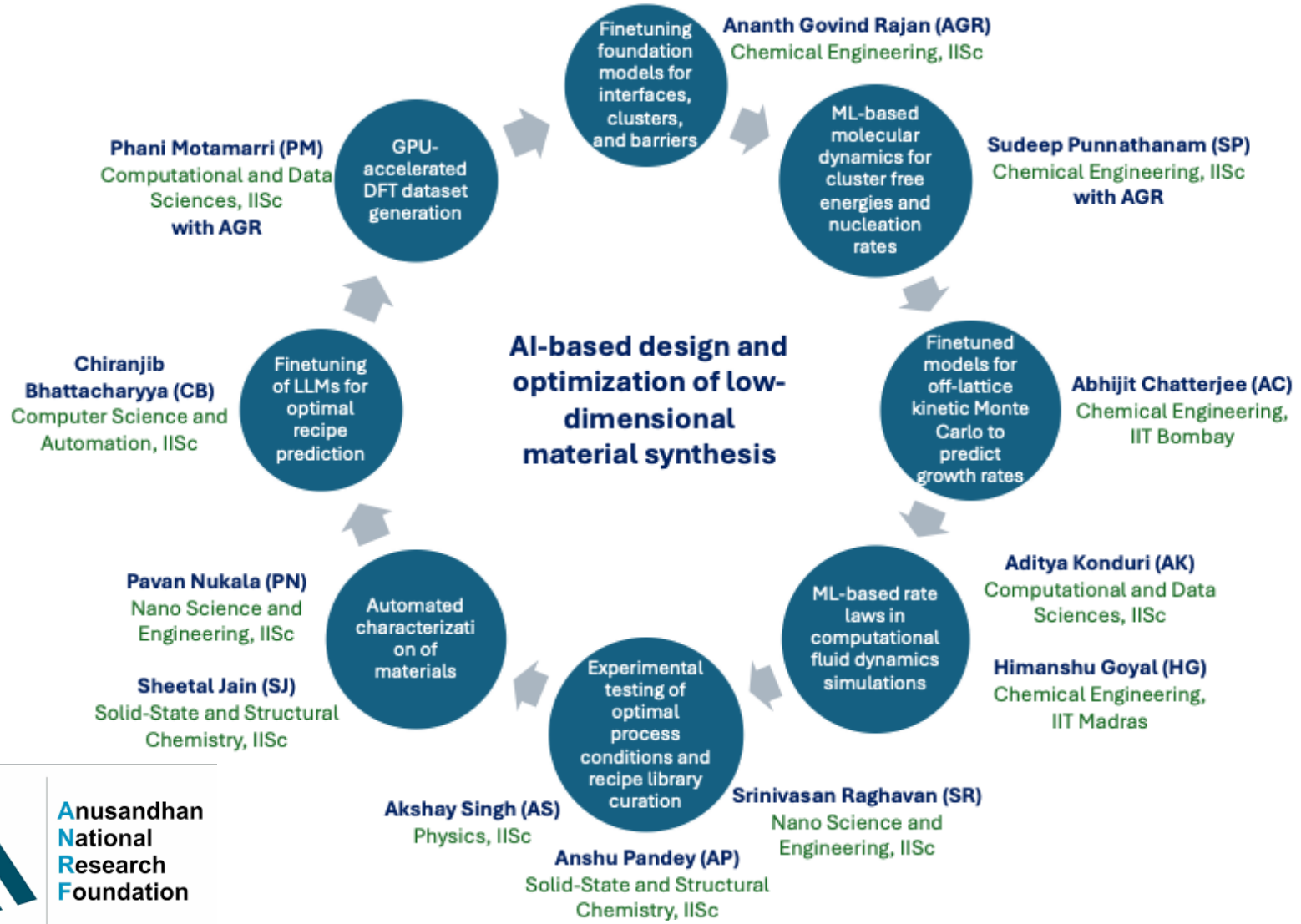
AI / ML for Materials Design

- Knowledge extraction to hypothesis formation to an “AI scientist”
- Globally: materials foundation models and generative design (e.g., MatterGen), knowledge graphs, and LLM-driven scientific workflows
- India: ANRF’s AI-for-Science mission + IndiaAI compute the start; fine-tuning vs. building indigenous models

Robotics for Automation

- Autonomous synthesis, characterization, and testing to close the loop
- Globally: A-Lab (Berkeley/LBNL), Acceleration Consortium (Toronto) show cycle times dramatically reducing
- India: need robotics-materials collaboration to yield mission-scale self-driving materials lab

Example: AI-aided Modeling and ACCelerated Experimentation for optimizing Low-dimensional MATerials synthesis (AIM-ACCELMAT)



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Summary

Strengths to build on

- Deep domain expertise across materials, catalysis, and computation at national institutes and labs
- Real national missions and funding already committed (carbon capture, semiconductors, critical minerals, batteries, etc.)
- Growing AI compute and robotics talent base

Gaps to work on

- No dedicated, mission-scale self-driving materials lab yet is a gap vs. A-Lab, Acceleration Consortium
- Fine-tuning vs. building indigenous foundation models
- Mission funding delivery lags targets (e.g., ACC PLI: ~1.4 of 50 GWh delivered)

Possible way forward

1. Pilot-scale self-driving materials labs at Indian institutes for specific application areas
2. Large-scale fine-tuned and custom-built materials foundation models, backed by shared compute and data
3. Accelerated-discovery approaches for named missions (magnets, batteries, semiconductors, catalysts, water)

Looking forward to Discussion 1.1: AI for scientific knowledge extraction: where does India stand? Fine-tuning existing LLMs, or building our own?

Acknowledgements

Anusandhan National Research Foundation

INDIAN INSTITUTE OF SCIENCE SERC

NSM NATIONAL SUPERCOMPUTING MISSION

हिन्दुस्तान पेट्रोलियम HP

Infosys Foundation

At IISc: Piyush Sharma | Sneha Thomas | Mahika Nair | Anand Verma | Shivam Chaturvedi | Swastik Paul Manas Sharma | Jampala Pasyanthi | Sudeep Punnathanam | Akshay Singh | Vivek Kumar | Srinibas Nandi Ambedkar Dukkipati | Rahul Sheshanarayana | Sayan Bhowmik

At HPCL: Kotni Santhosh | G Valavarasu

At A*STAR: Amol Amrute | Chuandayani Gwie | Pei Ying Moo | Chun Qi Joy Ng