

# SHIVAM CHATURVEDI

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## EDUCATION

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### Indian Institute of Science

Research Scholar (Ph.D.)

Chemical Engineering

Relevant Coursework: Machine Learning for Materials & Molecules (CH 251), Statistical Thermodynamics (CH 236), Nanotechnology (CH 241).

Bangalore, Karnataka

Aug 2022 - Present

### Malaviya National Institute of Technology

Bachelor of Engineering

Chemical Engineering

Cumulative GPA: 8.23/10

Relevant Coursework: Momentum Transfer Operations (CHT 203), Chemical Reaction Engineering (CHT 204), Chemical Engineering Thermodynamics (CHT 205)

Jaipur, Rajasthan

Aug 2018 - May 2022

## RESEARCH EXPERIENCE

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### Shell Technology Centre

Industry Project

**Advisors:** Amardeep Pathak (STC), Nishant Sinha (STC) & Ananth Govind Rajan

**Topic:** Unsteady State Microkinetic Modeling of electrochemical CO<sub>2</sub> reduction

- Developed & tested a **wrapper for MKMCXX**, optimizing it for **electrochemical CO<sub>2</sub> reduction reaction**.
- Built **microkinetic models** for reaction pathways & evaluated catalyst performance.

Bangalore, Karnataka

Apr 2023 – Nov 2024

### Chemical Engineering, MNIT

B. Tech. Thesis Project

**Advisors:** Madhu Agarwal (Chemical Engineering, MNIT)

**Topic:** Development of Bio-adsorbent for Arsenic Removal Using Hydrothermal Process

- Developed orange peel-based bio-adsorbents for arsenic removal from potable water in rural India
- Conducted adsorption studies & analyzed characterized material performance.

Jaipur, Rajasthan

Aug 2021 – Mar 2022

### IASc-INSANA-NASI

Summer Research Fellowship

**Advisors:** Venkatchalam Ramesh (Central University of Tamil Nadu)

**Topic:** Analyzing COVID-19 spread in the chest using CNN

- Designed a CNN-based X-ray analysis model to predict COVID-19 with 96.9% precision and 91.7% recall.
- Utilized ResNet & Transfer Learning for rapid and cost-effective disease detection.

Remote

Jun 2020 – July 2020

### Institute of Technology & Management, Salt Lake

Research Internship

**Advisors:** Satyasharan Changdar (ITM, Kolkata)

**Topic:** Predicting the viscosity of Various Nanofluids using the ANN

- Explored the new paradigm of Physics Guided Neural Network to get a generalized model that can predict nanofluids viscosity with high accuracy.

Remote

Aug 2020 – Feb 2021

## JOURNAL ARTICLES & PREPRINTS

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1. **Data-driven massive reaction networks reveal new pathways underlying catalytic CO<sub>2</sub> hydrogenation (In Review, Nature Communications)**

Anand M. Verma\*, **Shivam Chaturvedi\***, Swastik Paul\*, Srinibas Nandi, Rahul Sheshanarayana, Kotni Santhosh, G Valavarasu, Ambedkar Dukkipati, Chuandayani Gunawan Gwie, Pei Ying Moo, Chun Qi Joy Ng, Amol Amrute, Ananth Govind Rajan

[ChemRxiv preprint](#), 2025

2. **Advances in CO<sub>2</sub> Reduction on Bulk and Two-Dimensional Electrocatalysts: From First Principles to Experimental Outcomes**  
Raghavendra Rajagopalan\*, **Shivam Chaturvedi\***, Neeru Chaudhary\*, Abhijit Gogoi, Tej S Choksi, Ananth Govind Rajan  
[Current Opinion in Electrochemistry](#), 2025
3. **Transient Microkinetic Modeling and Reaction Network Representation of Electrochemical Mechanisms: Application to CO<sub>2</sub> Reduction and Oxygen Evolution (In Review, Advanced Theory and Simulations)**  
**Shivam Chaturvedi**, Amardeep Pathak, Nishant Sinha, Ananth Govind Rajan  
[ChemRxiv preprint](#), 2025
4. **Potential-Dependent Methane vs Methanol Selectivity During Electrochemical CO<sub>2</sub> Reduction on Al-Cu(111)/(211) via First-Principles Microkinetic Modeling (In preparation)**  
**Shivam Chaturvedi\***, **Abhijit Gogoi\***, Ananth Govind Rajan
5. **A Unique Physics-Aided Deep Learning Model for Predicting Viscosity of Nanofluids**  
Bivas Bhaumik, **Shivam Chaturvedi**, Satyasan Changdar, Soumen De  
[International Journal for Computational Methods in Engineering Science and Mechanics](#), 2023

## TEACHING EXPERIENCE

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<b>Machine Learning for Core Engineering Disciplines</b> Teaching Assistant with Prof. Ananth Govind Rajan	NPTEL, MOE Jul 2025 – Nov 2025
<b>Quantum-Mechanical Modelling of Nanomaterials (CH 253)</b> Teaching Assistant with Prof. Ananth Govind Rajan	Chemical Engineering, IISc Jan 2025 – May 2025
<b>Numerical Methods (CH 202)</b> Teaching Assistant with Prof. Narendra Dixit	Chemical Engineering, IISc Aug 2024 – Dec 2024
<b>Emerging Technologies in AI and ML (Faculty Development Programme)</b> Teaching Assistant with Prof. Ananth Govind Rajan	AICTE July 2024 – Nov 2024

## ACTIVITIES

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<b>INNOVATION COORDINATOR</b>	Institute Innovation Council, IISc (June 2024 - Present )
<b>CLUB CONVENOR, IISc HOCKEY CLUB</b>	IISc Gymkhana (Mar 2024 – Present)
<b>VICE PRESIDENT, CEA</b>	Chemical Engineering, IISc (Mar 2024 – Apr 2025)
<b>SOCIAL MEDIA SECRETARY, CEA</b>	Chemical Engineering, IISc (Mar 2023 – Apr 2024)
<b>CORE TEAM MEMBER, NATIONAL SERVICE SCHEME (NSS)</b>	MNIT (Aug 2019 – Mar 2021)
<b>EXECUTIVE MEMBER, ENERGY &amp; ENVIRONEMENT CLUB</b>	MNIT (Jan 2019 – Jan 2020)

## ADDITIONAL

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**Technical Skills:** HTML/CSS, MATLAB, Python, C++, Linux, Git  
**Modeling Tools:** VASP, VMD, ASE, Avogadro, MKMCXX, Blender,  
**Languages:** English, Hindi