Neeru Chaudhary

Postdoctoral Researcher, Nanyang Technological University, Singapore

Interests: Computational Catalysis for heterogeneous and electrochemical reaction, Alternative fuels, Machine learning, Functional Data Analysis

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EDUCATIONAL QUALIFICATION

B.E. (2007-11)
Chemical Engineering, Rajiv Gandhi Proudyogiki Vishwavidyalaya, India
Percentage: **72.59**

M. Tech (2011-13)
Chemical Engineering, Indian Institute of Technology, Roorkee, India
GPA: **8.68** **(A+ in dissertation)**

Ph. D. (2017-23)
Chemical Engineering, Washington State University, WA, USA
GPA: **3.52**

RESEARCH EXPERIENCE

Postdoctoral Researcher
School of Chemistry, Chemical Engineering and Biotechnology, **Nanyang Technological University, Singapore**
Dec. 2023 – Present

"Functional Data Modeling of Polymer Characterization Traces -Industry Collaboration with ExxonMobil"
- First-of-its-kind functional data analysis-based framework to model polymer structure–property relationships using full characterization traces (e.g., GPC, SAOS), enabling trace-to-trace predictions beyond scalar descriptors for inverse design via generative model (VAE, GANs) to improve design and testing.

"Redefining Catalysis Predictions Through Physics-Based Gaussian Model and Data-Driven Benchmarks for fuel cell application "
- Developed a machine learning-guided framework combining a bond-centric model for nanoparticle stability with Gaussian Process regression and OpenCatalyst models to reduce density functional theory computational cost and enable linking particle design to site-specific predictions for oxygen reduction reaction (ORR) catalytic performance.

"Confined Electrocatalytic Synthesis of Hydrogen Peroxide between Two Isolated Metal Sites"
- Investigated ORR activity and selectivity in metal–nitride (MN_4) doped graphene frameworks by modulating metal phthalocyanine (MPc) units, demonstrated enhanced two-electron transfer efficiency at dual-metal active sites.

Graduate Research Assistant (Ph. D.)
Voiland School of Chemical Engineering and Bioengineering, **Washington State University, WA, USA**
Aug. 2017- May 2023

Thesis: "Unraveling the Role of the Reaction Environment during Oxygenate Reduction from an Atomistic Perspective"
- Developed DFT-based models to investigate hydrodeoxygenation (HDO) of phenolics and hydrogenation of aldehydes pathways on transition metal surfaces- Pt, Ru, Fe, graphene and Fe_3C, incorporating coverage effects via mean-field model and Hamiltonian Lattice gas cluster expansion methods.
- Applied *Ab-initio* Molecular Dynamics (AIMD) simulations and proton–electron transfer (PET) mechanisms to study solvent effects; performed thermodynamic and kinetic analyses to evaluate catalytic performance and reaction pathways.

Project: "Hydrogenation of Carbon dioxide to formate via an ethyl carbonate intermediate during Carbon Capturing Process"
- Investigated hydrogenation of carbon dioxide to formate via an ethyl carbonate intermediate on Pd(111) in the presence of the ethanol solvent under the Eley-Rideal and Langmuir-Hinshelwood mechanism using DFT study.

Graduate Student (M. Tech.)
Chemical Engineering Department, **Indian Institute of Technology Roorkee, India**
Aug. 2011-Jul. 2013

Thesis: "Adsorptive Removal of Phenol from Synthetic Wastewater"
- Experimental research on simultaneous adsorption–biodegradation using aluminum-impregnated fly ash and *Pseudomonas putida*; conducted material characterization (SEM, BET, FTIR, XRD, FESEM, BET SA, TG/DTA and chemical analysis), optimized parameters using Response Surface Methodology (RSM) under Central composite rotary design (CCD) via Design Expert, and developed kinetic, equilibrium, and thermodynamic models for phenol removal.

Project: "Biological Production of Xylitol from Corn Husk and Switchgrass by Pichia stiptis"
- Produced xylitol through batch fermentation using *Pichia stipitis* on hydrolysates from corn husk, switchgrass, their mixture, and pure xylose; compared xylose uptake and xylitol yield after 72 h under optimized conditions.

CERTIFICATION

- **Google Advanced Data Analytics (full specialization),** *Google on Coursera*
- **Machine Learning (full specialization),** *DeepLearning.AI, Stanford University on Coursera*
- **Python for Data Science, AI & Development,** *IBM on Coursera*
- **Communication and Presentation skills,** *Naman Integrated Management Services Pvt. Ltd., India*
- **Licentiate of 3D TRASAR system Assurance Center,** *Nalco Water, An Ecolab Company*
- **Internship** *in Production Department of* **Indian Oil Corporation Ltd.**, *Panipat Refinery, India*
- **Internship** *in software training of AUTOCAD (Autodesk), AutoIso, AutoFlow, ProCAD, AFT Fathom, InstruCalc, PSVPlus at* **Neon Infotech Pvt. Ltd.**, *Indore, India*
- **Business English Certificate (Preliminary)** *conducted by University of Cambridge*

PROFESSIONAL & TEACHING EXPERIENCE

Technical Engineer III- SAC
NALCO WATER India Limited, India
Apr. 2016 - Jun. 2017

- Performed system audits, provided solutions to site engineer for optimized water utility; **high-ranking performer** in troubleshooting 3D TRASAR system alarms using tools and custom software (Toolbox, Envision, 3DT Optimize, TCO), installed at chemical units of NALCO's customer for cooling water, boiler, RO and membrane.

Faculty in Chemical Engineering Department
National Institute of Technology, Srinagar, India
Mar. 2015 - Jul. 2015

- Taught Thermodynamics-II and Process Instrumentation; handled labs in Mechanical Operations and Process Control for undergraduate students.

Associate System Engineer (SAP BASIS module)
IBM India Pvt. Ltd., India
Aug. 2013 – Nov. 2014

- Key contributor to a **successful GoLive** SAP ECC upgrade (4.6 to 6.0) for British Petroleum client as part of the BASIS team, responsible for system checks, patching, performance monitoring, and created production clones for post-GoLive support and issue resolution using SAP Notes.

SOFTWARE SKILLS

- **Machine learning**
- **VASP, Quantum ESPRESSO, ASE**
- **ATAT, NEB/CINEB, AIMD**
- **VESTA, VMD, OVITO, GNUPLOT**
- **MATERIAL STUDIO, MATERIAL PROJECTS**
- **Functional & Statistical Modeling**
- **LINUX/UINX, MATLAB, PYTHON**
- **DESIGN EXPERT**
- **AUTOCAD, AFT Fathom**
- **Microsoft Office, Excel**

AWARDS & ACHIEVEMENTS

- **Chair** *for Environmental and Automotive Catalysis in Catalysis and Reaction Engineering (CRE) Division of American Institute of Chemical Engineers (AIChE) (present)*
- Women in Engineering, Science, and Technology (**WiEST) Development Grant Awardee** *under the **Women in Technology (Micron)** category by NTU for leadership and innovation in STEM; awarded SGD 3,000 for professional development* (2025)
- **Top 10 Finalist** *for Poster presentation competition at Global Conference for Women Leaders and Emerging Researchers in Material Science (GLOW), NTU, Singapore (2024)*
- **Silver Award** *for Poster presentation at Singapore Catalysis Society (SCS) Forum (2024)*
- **Graduate Student Director** of *CRE Division of AIChE (2020-2022)*
- **Featured** *in WSU newsletter as an Inspiring Student (2020) https://vcea.wsu.edu/2020/04/09/inspiring-students/*
- **Hosted First Virtual Quarterly Student Research** *Symposium conducted by AIChE CRE division (2020)*
- **Honourable mention in Outstanding Student Recognition** from *International Precious Metal Education and Scientific Foundation (2021)*
- **Travel award** from *CRE division of AIChE (2019)*
- **Travel Award** from *Alaska Airlines (2018)*
- **Reviewer** *for reputed Journals- Industrial & Engineering Research Journal, Journal of Hazardous Materials, Chemical Engineering Communications, Chemistry and Ecology Journal, Desalination and Water Treatment, Separation Science and Technology (2014-present)*
- **6 Oral presentation** and **3 Poster presentation** *in various conferences- GLOW, SCS, AIChE, PCCS, JCDREAM (2018-present)*
- **Writing proposal** *for EMSL and progress report for DOE with Advisor at WSU, USA (2018-2022)*
- **Volunteer** *for ChEGSA Event at WA Eastern Regional Science Olympiad Tournament (2018-2019)*
- **Volunteer** *at AIChE Graduate Recruitment Fair (2018)*
- **Assistantship** from *Ministry of Human Resource Development (MHRD), Government of India, IITR (2011-13)*
- **Training Co-ordinator** *at Institute of Technology and Management (ITM), M.P., India (2010)*

ADDITIONAL EXPERIENCE

- Attended online workshop on The Past, Present, and Future for Forcefield led conducted by Materials Design (2023)
- Attended online workshop on Introduction to DFT for experimentalist & latest advances led by PARADIM summer school, Cornell University (2023)
- Attended virtual workshop on Machine Learning for Materials Bootcamp conducted by University of Madison (2023)
- Attended virtual workshop on Computational Chemistry and Materials Science (CCMS) by summer institute at the Lawrence Livermore National Laboratory (2020)
- Attended soft skills training conducted by Hewlett-Packard (HP) at ITM university (2010)
- Field experience in KS Oil refinery, Morena, Madhya Pradesh, India (2009)

LIST OF PUBLICATION

- Chuhong Lin, Bryan C. S. Lee, Uzma Anjum, Asmese M. Prabhu, **Neeru Chaudhary**, Rong Xu, and Tej S. Choksi, Harnessing Physics-inspired Machine Learning to Design Nanocluster Catalysts for Dehydrogenating Liquid Organic Hydrogen Carriers, *Appl. Catal. B-Environ. Energy,* 2025, 371, 125192.
- Raghavendra Rajagopalan, Shivam Chaturvedi, **Neeru Chaudhary**, Abhijit Gogoi, Tej S. Choksi and Ananth Govind Rajan, CO_2 Reduction Thermodynamics and Kinetics on Bulk and Two-Dimensional Electrocatalysts: From First Principles to Experimental Outcomes*, Curr. Opin. Electrochem*., 2025, 51, 101668 .
- Alyssa J.R. Hensley, **Neeru Chaudhary,** Naseeha Cardwell, Isaac Onyango, Yong Wang, Di Wu, Jean-Sabin McEwen, Capturing Surface Coverage Effects In Heterogeneous Catalysis*, J. Phys. Chem. C*., 2024, 129, 1907-1929, with **Front Cover** and **Authors biography**.
- **Neeru Chaudhary**, Isaac Onyango, Yong Wang and Jean-Sabin McEwen, Determining Catalytically Relevant Surfaces through Coverage-Dependent Lattice Gas Models: Carbon Adsorption on Fe(100), *J. Phys. Chem. C.,* 2023, 127, 14163-14176 with **Cover art.**
- Xianghui Zhang, **Neeru Chaudhary**, Megan R. Hawkins, Cody B. Cockreham, Chen Yang, Junnan Shangguan, Alyssa J. R. Hensley, Ya-Huei Cathy Chin, Su Ha, Jean-Sabin McEwen and Di Wu, Determining the hydration energetics on carbon-supported Ru catalysts: An adsorption calorimetry and density functional theory study, *Catal. Today.* 2021, 365, 172-180.
- **Neeru Chaudhary**, Alyssa Hensley, Greg Collinge, Yong Wang and Jean-Sabin McEwen, Coverage-Dependent Adsorption of Phenol on Pt(111) from First Principles, *J. Phys. Chem. C.,* 2020, 124, 356-362 with **Cover art.**
- **Neeru Chaudhary*,** Chandrajit Balomajumder, Bhumica Agrawal, Vidyasagar Jagati, Removal of Phenol Using Fly Ash and Impregnated Fly Ash: An Approach to Equilibrium, Kinetic, and Thermodynamic Study, *Sep. Sci. Technol.,*2015, 50, 690-699.
- **Neeru Chaudhary*,** Chandrajit Balomajumder, Optimization study of adsorption parameters for removal of phenol on aluminum impregnated fly ash using response surface methodology, *J. Taiwan Inst. Chem. Eng.*, 2014, 45, 852–859.
- **Neeru Chaudhary*,** Chandrajit Balomajumder, Vidyasagar Jagati, Biological Production of Xylitol from Corn Husk and Switchgrass by *Pichia stiptis*, *Res. J. Chem. Sci.*, 2013, 3, 58-64.

Underlined- first co-author; Asterisk (*) corresponding author