Nikhil R. Agrawal - Curriculum Vitae

Process Engineer 3
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EDUCATION

Ph.D. in Chemical Engineering

August 2018 - August 2024

University of California, Berkeley, USA

Advisor: Prof. Rui Wang

Thesis title: Modified Gaussian Renormalized Fluctuation Theory for Electrolytes at Interfaces

Thesis committee: David T. Limmer, Kranthi K. Mandadapu, and Clayton J. Radke

B.S. and M.S. (Dual Degree) in Chemical Engineering Indian Institute of Technology (IIT), Delhi, India

July 2013 - July 2018

Master's thesis title: Minkowski Tensors to Characterize Particle Packings in Packed Bed Reactors

Master's thesis advisor: Prof. Shantanu Roy Institute medal for highest GPA in the program

WORK EXPERIENCE

Designing high throughput processes for synthesis of novel thin film materials Oct '24 - Present Process Engineer 3 | Deposition Product Group, Lam Research, Oregon, USA

- Identify and screen new processes for commercially feasibly manufacturing of thin films
- Engineer and optimize hardware configuration of chemical reactors
- Ensure smooth integration of the new process with existing processes in semiconductor manufacturing
- Engage with Lam's customers to understand their needs and accommodate them into business strategy of Lam

Thermodynamics and transport modeling of electrolytes at interfaces Ph.D. Candidate | Mentor: Prof. Rui Wang, UC Berkeley, California, USA

Aug '18 - Aug '24

Deep Gaussian Processes for uncertainty quantification of machine-learned free energies Mar '24 - June '24 Research Intern |, Lawrence Livermore National Laboratory, California, USA

Hybrid Kinetic Monte-Carlo and MD simulations to study mitotic spindle formation June '23 - Aug '23 Summer Predoctoral Researcher | Flatiron Institute, New York, USA

Microscopic characterization of particle packings in packed bed reactors

Master's Candidate | Mentor: Prof. Shantanu Roy, Chemical Engineering, IIT Delhi, India

Sequential Particle Deposition to simulate overdamped granular systems

May '17 - July '17

Visiting Researcher | Mentor: Prof. Dr. Thorsten Pöschel University of Erlangen-Nuremberg, Germany

Image processing and pore network modeling for multiphase flows in porous media

May '16 - July '16

Summer Intern | Mentor: Dr. Paul Duru, Institut de Mecanique des Fluides de Toulouse (IMFT), France

Design and characterization of visible light photo-catalysts for CO₂ reduction May'15 - April '16 Undergraduate Researcher | Mentor: Prof. Suddhasatwa Basu, Chemical Engineering, IIT Delhi, India

JOURNAL PUBLICATIONS AND PREPRINTS

- 1. Electrostatic Correlation Augmented Self-Consistent Field Theory and Its Application to Polyelectrolyte Brushes
 - Chao Duan, Nikhil R. Agrawal, and Rui Wang, Physical Review Letters (2025) 134, 048101
- 2. Understanding long-range opposite-charge repulsion in multivalent salt solutions **Nikhil R. Agrawal**, Carlo Carraro and Rui Wang, J. Chem. Phys. 161, 204902 (2024)
- 3. Nature of overcharging and charge inversion in electrical double layers

 Nikhil R. Agrawal, Chao Duan, and Rui Wang, J. Phys. Chem. B 2024, 128, 1, 303–311
- Ion correlation-driven like-charge attraction in multivalent salt solutions
 Nikhil R. Agrawal, Ravtej Kaur, Carlo Carraro and Rui Wang, J. Chem. Phys. 159, 244905 (2023)
- 5. Non-monotonic salt concentration dependence of inverted electrokinetic flow **Nikhil R. Agrawal** and Rui Wang, *AIChE Journal*, e18269, 2023.
- Self-consistent description of vapor-liquid interface in ionic fluids
 Nikhil R. Agrawal and Rui Wang, Physical Review Letters (2022), 129, 228001.
- 7. Electrostatic correlation induced ion condensation and charge inversion in multivalent electrolytes

 Nikhil R. Agrawal and Rui Wang, Journal of Chemical Theory and Computation (2022), 18, 6271-6280
- 8. A first-order segregation phenomenon in fluid-immersed granular systems
 Prapanch Nair, LAT Cisneros, CRK Windows-Yule, **Nikhil R. Agrawal**, Shantanu Roy, and Thorsten
 Pöschel, *Powder Technology* 373 (2020): 357-361.
- 9. Isotropy of sphere packings in a cylindrical confinement Nikhil R. Agrawal, Prapanch Nair, Thorsten Pöschel and Shantanu Roy, Chemical Engineering Journal 377 (2019): 119820.

In preparation:

10. Sturm–Liouville theory inspired method to solve the Modified Gaussian Renormalized Fluctuation theory for electrolytes

Nikhil R. Agrawal, Carlo Carraro and Rui Wang.

COURSEWORK AND CERTIFICATIONS

- Bayesian Data Analysis and Machine Learning for Physical Sciences
- Machine Learning, Statistical Models, and Optimization for Biological and Chemical Problems
- Statistical Thermodynamics & Transport Phenomena
- Finite Element Methods
- Numerical Methods in Chemical Engineering

- Fundamentals of Deep Learning (NVIDIA)
- Data Parallelism: How to Train Deep Learning Models on Multiple GPUs (NVIDIA)
- Model Parallelism: Building and Deploying Large Neural Networks (NVIDIA)
- Chemical Reaction Engineering I and II
- Fundamentals of Computational Fluid Dynamics

SELECTED PRESENTATIONS

1. Beyond mean-field Poisson-Boltzmann: A self-consistent theory for electrical double layers 2023 American Physical Society March Meeting, Poster Presentation

- 2. A self-consistent theory for complex electrostatic phenomena at interfaces 2022 American Chemical Society Colloid and Surface Science Symposium, Oral Presentation
- 3. Ion correlation induced non-monotonic height change and microphase separation of polyelectrolyte brushes 2024 American Physical Society March Meeting, Oral Presentation
- 4. Electrostatic wetting transition: charge inversion and like charge attraction 2021 American Chemical Society Colloid and Surface Science Symposium, Oral Presentation
- 5. Correlation Induced Electrostatic Wetting and Charge Inversion
 2020 American Institute of Chemical Engineers Annual Meeting, Oral Presentation

AWARDS AND HONOURS

- Langmuir Graduate Student Oral Presentation Awards Finalist, American Chemical Society 2022
- Institute Silver Medal from IIT Delhi for highest GPA in the dual degree program in Chemical Engg. 2018
- IIT Delhi Semester Merit Award for 9 out of 10 semesters for being among top 7% meritorious students across the dual degree program, consecutively for 8 semesters 2013-2017
- Significant Contribution to Research Activities Award by Chemical Engineering Society, IIT Delhi 2017
- Kishore Vaigyanik Protsahan Yojana (KVPY) Fellowship by Department of Science and Technology, Govt. of India 2013
- Was among the *Nation's Top 1*% merit holders in National Standard Examination in Physics (NSEP) conducted by the Indian Association of Physics Teachers (IAPT)

ACADEMIC ADVISING

- Julien Kehon, Undergraduate majoring in Chemical Engg. at UC Berkeley (Jan 2022 May 2022)
- Ravtej Kaur, Undergraduate majoring in Chemical Engg. at UC Berkeley (Jan 2023 August 2023)

SERVICE & OUTREACH

Secretary, SPIC MACAY, IIT Delhi

April '15 - April '16

SPIC MACAY: Society for Promotion of Indian Classical Music And Culture Amongst Youth

Led a team of 13 to organize marketing, publicity, and hospitality of club events like dance workshops and music concerts for eminent artists including Grammy Awardee Pt. Vishwa Mohan Bhatt.

SKILLS

Domain Knowledge Process Design, Thermodynamics, Transport Phenomena, Applied Machine

Learning, Computational Modeling

Programming Skills Pyth

Python, C++, PyTorch, GPyTorch, TensorFlow, Scikit Learn, Bash

Technical software

JMP, MATLAB, Aspen, COMSOL, FLUENT, ParaView, Autodesk Inventor

Languages English and Hindi

HOBBIES AND INTERESTS

Sociology, Psychology, listening to classical music, and a keen interest in philosophical discussions