# Nikhil R. Agrawal - Curriculum Vitae

Process Engineer 3 Deposition Product Group, Lam Research Building C, 11355 SW Leveton Drive Tualatin, OR, USA 97062

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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

## RESEARCH EXPERIENCE

# Plasma Enhanced Atomic Layer Deposition (PEALD) processes

Oct '24 - Present

Process Engineer 3 | Deposition Product Group

Lam Research, Tualatin, Oregon, USA

### Thermodynamics and transport modeling of electrolytes at interfaces

Aug '18 - Present

Ph.D. Candidate | Mentor: Prof. Rui Wang

Pitzer Center for Theoretical Chemistry, UC Berkeley, California, USA

## Deep Gaussian Processes for uncertainty quantification of machine-learned free energies Mar '24 - June '24 Research Intern | Mentor: Dr. Amit Samanta

Physics & Materials Science Division, 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 | Mentor: Dr. Adam R. Lamson and Prof. Michael J. Shelley

Center for Computational Biology, Flatiron Institute, New York, USA

## Microscopic characterization of particle packings in packed bed reactors

Jan '17 - July '18

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

#### Sequential Particle Deposition to simulate overdamped granular systems

May '17 - July '17

Visiting Researcher | Mentor: Prof. Dr. Thorsten Pöschel

Institute of Multi-scale Simulations (MSS), University of Erlangen-Nuremberg, Germany

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

May '16 - July '16

Summer Research Associate | Mentor: Dr. Paul Duru

Institut de Mecanique des Fluides de Toulouse (IMFT), Toulouse, France

## Design and characterization of visible light photo-catalysts for CO<sub>2</sub> reduction

May'15 - April '16

Undergraduate Researcher | Mentor: Prof. Suddhasatwa Basu

Department of Chemical Engineering, IIT Delhi, India

#### JOURNAL PUBLICATIONS AND PREPRINTS

- 1. Understanding long-range opposite-charge repulsion in multivalent salt solutions Nikhil R. Agrawal, Carlo Carraro and Rui Wang, under review, arXiv:2408.15520.
- 2. Electrostatic Correlation Augmented Self-Consistent Field Theory and Its Application to Polyelectrolyte Brushes
  - Chao Duan, Nikhil R. Agrawal, and Rui Wang, under review, arXiv:2404.09103.
- 3. Nature of overcharging and charge inversion in electrical double layers

  Nikhil R. Agrawal, Chao Duan, and Rui Wang, The Journal of Physical Chemistry 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, The Journal of Chemical Physics 159, 244905 (2023)
- 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** Computational Modeling, Thermodynamics, Transport Phenomena, Applied Machine

Learning, Finite Difference, Finite Element, and Spectral Methods

Programming Skills Technical software Python, C++, PyTorch, GPyTorch, TensorFlow, Scikit Learn, Bash ParaView, MATLAB, COMSOL, FLUENT, Autodesk Inventor

Languages English and Hindi

## HOBBIES AND INTERESTS

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