Nikhil R. Agrawal - Curriculum Vitae

Ph.D. Candidate
Department of Chemical and Biomolecular Engineering
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EDUCATION

Ph.D. in Chemical and Biomolecular 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*

B.S. and M.S. (Dual Degree) in Chemical Engineering July 2013 - July 2018
Indian Institute of Technology (IIT), Delhi, India
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

Statistical physics of concentrated 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 Roy
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_2 reduction *May'15 - April '16*
Undergraduate Researcher | Mentor: Prof. Suddhasatwa Basu
Department of 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, *under review*, *arXiv:2404.09103.*

2. 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*

3. Ion correlation-driven like-charge attraction and reentrant condensation in multivalent salt solutions
Nikhil R. Agrawal, Ravtej Kaur, Carlo Carraro and Rui Wang, *The Journal of Chemical Physics 159, 244905 (2023)*

4. Non-monotonic salt concentration dependence of inverted electrokinetic flow
Nikhil R. Agrawal and Rui Wang, *AIChE Journal, e18269, 2023.*

5. Self-consistent description of vapor-liquid interface in ionic fluids
Nikhil R. Agrawal and Rui Wang, *Physical Review Letters (2022), 129, 228001.*

6. 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*

7. 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.*

8. 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:

9. Long-range opposite-charge repulsion in multivalent salt solutions
Nikhil R. Agrawal, Carlo Carraro and Rui Wang.

10. Sturm–Liouville theory inspired approach to solving Gaussian ion-ion correlation functions
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 Mechanics & 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)
- Partial Differential Equations
- Fundamentals of Computational Fluid Dynamics

SELECTED PRESENTATIONS

1. Beyond mean-field Poisson-Boltzmann: A self-consistent theory for electrical double layers
Energy Conversion Group, Lawrence Berkeley National Laboratory, **Invited Presentation**, *Feb 2023*

2. Modified Gaussian Renormalized Fluctuation theory: A self-consistent electrolyte solution theory
Pitzer Center for Theoretical Chemistry, **Invited Presentation**, *Jan 2023*

3. Self-consistent theory to describe charge inversion and like-charge attraction in multivalent electrolytes
   2023 American Physical Society March Meeting, Oral Presentation
4. A self-consistent theory for complex electrostatic phenomena at interfaces
   2022 American Chemical Society Colloid and Surface Science Symposium, Oral Presentation
5. Vapor-Liquid interface in ionic fluids
   2022 American Physical Society March Meeting, Oral Presentation
6. Ion correlation induced non-monotonic height change and microphase separation of polyelectrolyte brushes
   2024 American Physical Society March Meeting, Oral Presentation
7. 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) 2013

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