

# Nikhil R. Agrawal - Curriculum Vitae

Ph.D. Candidate

Department of Chemical and Biomolecular Engineering  
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## EDUCATION

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**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*

**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

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**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<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

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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](https://arxiv.org/abs/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

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|---|---|
| • Bayesian Data Analysis and Machine Learning for Physical Sciences                           | • Fundamentals of Deep Learning (NVIDIA)  |
| • Machine Learning, Statistical Models, and Optimization for Biological and Chemical Problems | • Data Parallelism: How to Train Deep Learning Models on Multiple GPUs (NVIDIA) |
| • Statistical Mechanics & Transport Phenomena   | • Model Parallelism: Building and Deploying Large Neural Networks (NVIDIA)      |
| • Finite Element Methods  | • Partial Differential Equations  |
| • Numerical Methods in Chemical Engineering   | • Fundamentals of Computational Fluid Dynamics                                  |

## SELECTED PRESENTATIONS

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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

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- 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

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- 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

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### 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

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<b>Domain Knowledge</b>	Computational Modeling, Thermodynamics, Transport Phenomena, Applied Machine Learning, Finite Difference, Finite Element, and Spectral Methods
<b>Programming Skills</b>	Python, C++, PyTorch, GPyTorch, TensorFlow, Scikit Learn, Bash
<b>Technical software</b>	ParaView, MATLAB, COMSOL, FLUENT, Autodesk Inventor
<b>Languages</b>	English and Hindi

## HOBBIES AND INTERESTS

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