

# Pavan Ravindra

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## RESEARCH EXPERIENCE

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**Columbia University - Reichman Group** 2022-Present  
Advisor: David Reichman *PhD Student*

- **Dynamic Mode Decomposition (DMD):** Applies DMD to probe long timescale behaviors of molecular dynamics simulations
- **Glassy Systems:** Uses numerical methods to study the glass transition in supercooled liquids

**Brookhaven National Laboratory** Summer 2024  
Advisor: Deyu Lu *Visiting Student*

- **Machine Learning for XAS:** Used machine learning to extract physical descriptors of metal oxides from experimental x-ray absorption spectroscopy data

**University of Cambridge - ICE Group** 2021-2022  
Advisor: Angelos Michaelides *Master's Student*

- **Machine Learning Potentials:** Used committees of neural network potentials to accelerate chemical simulations at the accuracy of *ab initio* calculations
- **Nanomaterial Characterization:** Applied machine learning, molecular dynamics, and density functional theory calculations to characterize phase transitions and chemical properties of two-dimensional nano-confined water

**University of Maryland - Tiwary Group** 2018-2021  
Advisor: Pratyush Tiwary *Undergraduate Researcher*

- **Simulations of Biomolecules:** Used molecular dynamics simulations to characterize the kinetics and thermodynamics of biomolecules, primarily protein-ligand systems
- **Information Theory:** Developed, tested, and applied an information theoretic algorithm to identify a basis set of order parameters for collective variable construction

## EDUCATION

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**Columbia University** 2022-Present  
*PhD in Chemical Physics* GPA: 4.11/4.00

**University of Cambridge** 2021-2022  
*MPhil in Chemistry* Churchill Scholarship

**University of Maryland, College Park** 2017-2021  
*B.S. in Biochemistry, B.S. in Computer Science* GPA: 3.99/4.00

## PUBLICATIONS

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**Ravindra, P.**, Advincula, X. R., Schran, C., Michaelides, A., Kapil, V. (2023). A quasi-one-dimensional hydrogen-bonded monolayer ice phase. *arXiv*.

Smith, Z., **Ravindra, P.**, Wang, Y., Cooley, R., Tiwary, P. (2020). Discovering Protein Conformational Flexibility Through Artificial Intelligence Aided Molecular Dynamics. *The Journal of Physical Chemistry B*.

**Ravindra, P.**, Smith, Z., Tiwary, P. (2020). Automatic mutual information noise omission (AMINO): Generating order parameters for molecular systems. *Molecular Systems Design & Engineering*.

## AWARDS

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- **Jack Miller Teaching Award (2024)** - given to ~6 graduate students in the Columbia chemistry department annually to recognize excellence in teaching
- **Department of Energy Computational Science Graduate Fellowship (DOE CSGF) (2022)** - provides full PhD funding for students involved in computationally-intensive research
- **Churchill Scholarship (2021)** - given to 16 students in the US annually to fund a year of study at the University of Cambridge towards a master's degree
- **Goldwater Scholarship (2020)** - a national scholarship for recognizing undergraduate research in the natural sciences, engineering, and mathematics
- **Banneker/Key Scholarship (2017)** - a 4-year merit scholarship offered to incoming University of Maryland undergraduates to fully fund college expenses

## TEACHING EXPERIENCE

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### Teaching Assistant - Chemistry

Spring 2023, Spring 2024

*CHEM 1404 - General Chemistry II (Columbia University)*

- Planned weekly 50 minute recitations to review lecture material and solve practice problems
- Designed and wrote quizzes for students.
- Average rating from students: 4.78/5.00 from 45 responses (reviews available upon request)

### Head Teaching Assistant - Computer Science

Fall 2019 - Spring 2021

*CMSC330 - Organization of Programming Languages (University of Maryland)*

- Managed a team of ~35 TAs to organize one of the largest computer science courses at the University of Maryland (500+ students per semester)
- Organized and coordinated weekly TA meetings to assign duties to other TAs
- Designed and wrote projects, exams, and quizzes for students

### Teaching Assistant - Chemistry

Spring 2019 - Spring 2021

*CHEM242 - Organic Chemistry II Lab (University of Maryland)*

- Directed weekly laboratory activities for a group of 18 undergraduate students
- Graded assignments and exams

## MISCELLANEOUS

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### Competitive Rubik's Cube Speedsolving

- Formerly ranked 4th in the world for fastest time solving a Rubik's cube [[video link](#)]
- Peak ranking of 2nd in the world for one-handed Rubik's cube
- Set 5 US national records

### Rubik's Cube Competition Organizer

- Organizes competitions that attract 200+ international competitors
- Organized CubingUSA Northeast Championship 2019, the regional championship for the World Cube Association for the northeast US region