Avishek Das, Postdoctoral Researcher

Contact Information

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Research Interests

Information processing in soft matter, Biophysics of cellular motility, Nonequilibrium self-organization in colloids, Rare event sampling, Numerical algorithms for statistical physics

Current Position

FOM Institute for Atomic and Molecular Physics (AMOLF), Amsterdam, The Netherlands

Postdoctoral researcher, Sep 2022-Now

- Adviser: prof. dr. Pieter Rein ten Wolde
- Quantifying directional information transfer in the signaling network for bacterial chemotaxis

Education

University of California, Berkeley, United States

Ph.D., Physical Chemistry, Aug 2017-May 2022

- Adviser: Prof. David Limmer
- Sampling rare fluctuations in nonequilibrium trajectories with optimal control forces, applications to inverse design of self-assembly

Indian Institute of Science, Bangalore, India

B.Sc.(Research), Chemistry(Major), Physics(Minor), Aug 2013-May 2017

- Adviser: Prof. D. D. Sarma
- Electronic structure of strongly correlated transition metal oxides using MP2 theory

Other Research Experience

Fritz-Haber Institute of Max-Planck Society, Berlin, Germany

- Adviser: Dr. Luca M. Ghiringhelli
- Implementation of electron localization descriptors in an all-electron full-potential electronic structure code with numeric atom-centered basis functions (2016)

Indian Institute of Technology Bombay, Mumbai, India

- Adviser: Prof. Gopalan Rajaraman
- Ab-initio computational investigation of dependence of magnetic anisotropy of tetrahedral mononuclear Co(II) complexes on structural distortion and ligand environment (2015)

Indian Institute of Science, Bangalore, India

- Adviser: Prof. P. S. Mukherjee
- Planned supramolecular self-assembly of co-ordination based nanocages and their use in catalysis of organic reactions (2014-15)

Indian Institute of Science, Bangalore, India

- Adviser: Prof. Santanu Bhattacharya

- pH-sensitive aqueous self-assembly of small(tri- and tetra-) peptides and functionalizations for use as drug delivery vehicle (2014)

Technical Skills

- Python, C, C++, FORTRAN, Julia, MATLAB, Mathematica
- LAMMPS, Gaussian09, MOLCAS, ORCA, FHI-AIMS, Q-CHEM

Awards

APS March Meeting
- Best Student Speaker Award (Statistical & Nonlinear Physics), 2022

Kavli Energy Nanoscience Institute, UC Berkeley
- Philomathia Graduate Student Fellow, 2021

College of Chemistry, UC Berkeley
- College of Chemistry Graduate Diversity Program Award, 2021

Graduate Division, UC Berkeley
- Outstanding Graduate Student Instructor Award, 2019

Indian Institute of Science, Bangalore
- Institute gold medal for best performance, 2017

German Academic Exchange Service
- Working Internships in Science and Engineering (WISE) Fellow, 2016

Indian Academy of Sciences
- Summer Research Fellow, 2015

8$^{\text{th}}$ Asian Science Camp, NTU Singapore
- Member of Indian delegation, 2014

45$^{\text{th}}$ International Chemistry Olympiad, Moscow
- Silver medal, 2013

Indian National Olympiads
- Gold medals in chemistry and biology, 2013

Dept. of Science and Technology, Govt. of India
- Basic Science Fellow, 2013

Publications

* = corresponding author; † = equal contribution

[1] A. N. Singh*, **A. Das*** and D. T. Limmer*, Variational path sampling of rare dynamical events, *Annu. Rev. Phys. Chem.*, 76, 639-662 (2025), DOI

[2] **A. Das*** and P. R. ten Wolde*, Exact computation of transfer entropy with Path Weight Sampling, arXiv:2409.01650 (2024), arXiv

[3] C. P. N. Tanner, V. Wall, J. Portner, **A. Das**, J. K. Utterback, A. Jeong, M. Gababa, I. Coropceanu, L. Hamerlynck, J. Raybin, M. J. Hurley, N. Leonard, A. Kim, C. J. Tassone, A. Fluerasu, Y. Sun, D. T. Limmer, S. W. Teitelbaum, D. V. Talapin and N. S. Ginsberg, Enhancing nanocrystal superlattice self-assembly near a metastable liquid binodal, *accepted: Nature Physics* (2025), arXiv

[4] C. P. N. Tanner, J. K. Utterback, J. Portner, I. Coropceanu, **A. Das**, C. J. Tassone, S. W. Teitelbaum, D. T. Limmer, D. V. Talapin and N. S. Ginsberg, In situ X-ray scattering reveals coarsening rates of superlattices self-assembled from electrostatically stabilized metal nanocrystals depend nonmonotonically on driving force, *ACS Nano*, 18, 7, 5778-5789 (2024), DOI

[5] M. J. Hurley, C. P. N. Tanner, J. Portner, J. K. Utterback, I. Coropceanu, G. J. Williams, **A. Das**, A. Fluerasu, Y. Sun, S. Song, L. M. Hamerlynck, A. H. Miller, P. Bhattacharyya, D. V. Talapin, N. S. Ginsberg and S. W. Teitelbaum, In situ coherent X-ray scattering reveals polycrystalline structure and discrete annealing events in strongly coupled nanocrystal superlattices, *Physical Review Research*, 6, 023119 (2024), DOI

[6] **A. Das** and D. T. Limmer, Nonequilibrium design strategies for functional colloidal assemblies, *Proceedings of the National Academy of Sciences*, 120 (40), e2217242120 (2023), DOI

[7] R. Clune†, **A. Das**†, D. Jasrasaria†, E. Rossomme, O. Cohen, and A. M. Baranger, Development of a week-long mathematics intervention for incoming chemistry graduate students, *Journal of Chemical Education*, 100, 3291-3301 (2023), DOI

[8] I. Coropceanu, E. Janke, J. Portner, D. Haubold, N. Trung, **A. Das**, C. Tanner, J. Utterback, S. Teitelbaum, M. Hudson, N. Sarma, A. Hinkle, C. Tassone, A. Eychmüller, D. T. Limmer, M. Olvera de la Cruz, N. S. Ginsberg and D. Talapin, Self-assembly of nanocrystals into strongly electronically coupled all-inorganic supercrystals, *Science*, 375, 1422–1426 (2022), DOI

[9] **A. Das**†, B. Kuznets-Speck† and D. T. Limmer, Direct evaluation of rare events in active matter from variational path sampling, *Physical Review Letters*, 128, 028005 (2022), DOI

[10] **A. Das**†, D. Rose†, J. P. Garrahan and D. T. Limmer, Reinforcement learning of rare diffusive dynamics, *Journal of Chemical Physics*, 155, 134105 (2021), DOI

[11] **A. Das**, and D. T. Limmer, Variational design principles for nonequilibrium colloidal assembly, *Journal of Chemical Physics*, 154, 014107 (2021), DOI

[12] **A. Das**, and D. T. Limmer, Variational control forces for enhanced sampling of nonequilibrium molecular dynamics simulations, *Journal of Chemical Physics*, 151, 244123 (2019), DOI

Talks

† = invited.

Utility of information for stochastic navigators

- NWO Biophysics annual conference, Veldhoven, The Netherlands, Oct 2025

Exact computation of transfer entropy with Path Weight Sampling

- StatPhys29, Florence, Italy, Jul 2025
- NWO Physics annual conference, Veldhoven, The Netherlands, Jan 2025

Quantifying directional information flow in bacterial signaling with a new importance sampling technique

- †Pitzer Center for Theoretical Chemistry seminar, UC Berkeley, Apr 2024

Utility of biochemical information flow in bacterial chemotaxis

- †Arago Physics of Life symposium, University of Twente, Apr 2024
- †Kavli ENSI 10 year anniversary symposium, UC Berkeley, Apr 2024
- Physical Biology Circle Meeting, Instituto Gulbenkian de Ciência, Lisbon, Feb 2024
- NWO Biophysics annual conference, Veldhoven, The Netherlands, Oct 2023
- Physics of Microbial Motility workshop, University of Würzburg, Würzburg, Oct 2023

Variational sampling of rare nonequilibrium trajectories

- †Solid State and Structural Chemistry seminar, Indian Institute of Science, Bangalore, Sep 2023

Designing autonomous functional self-assembly in nonequilibrium

- †Computational Soft Matter seminar, University of Amsterdam, Amsterdam, Jun 2023
- †Programmable Matter seminar, ESPCI, Paris, *virtual*, Nov 2022

Direct evaluation of rare events in active matter from variational path sampling

- CECAM workshop: Numerical Techniques for Nonequilibrium Steady States, Mainz, Apr 2022
- †Pitzer Center for Theoretical Chemistry seminar, UC Berkeley, Apr 2022
- *APS March Meeting, Chicago, Mar 2022
  ***Best student speaker award**, Topical Group on Statistical and Nonlinear Physics

Nonequilibrium response in molecular simulations, I & II

- †Summer School: Advanced Cyberinfrastructure Training for Modeling Physical Systems, Rensselaer Polytechnic Institute, New York, *virtual*, Jul 2021

Optimal driving forces for reweighting trajectory ensembles

- CECAM workshop: Numerical Techniques for Nonequilibrium Steady States, *digital prequel*, May 2021

Automated discovery of design principles for far-from-equilibrium colloidal self-assembly

- Middle European Cooperation in Statistical Physics, *virtual*, May 2021

Variational inverse design for nonequilibrium colloidal self-assembly

- APS March Meeting, *virtual*, Mar 2021

Nonequilibrium variational control forces for self-limited colloidal assembly

- APS March Meeting *(conference cancelled)*, Denver, Mar 2020

Variational estimation of large deviation functions

- Berkeley Statistical Mechanics Breakout Meeting, UC Berkeley, Jan 2019

Posters

Exact computation of transfer entropy with Path Weight Sampling

- Information in Matter symposium, AMOLF, Amsterdam, May 2025
- NWO Biophysics annual conference, Veldhoven, The Netherlands, Oct 2024

Performance benefit of information in chemotaxis

- Theory and Concepts in Biology symposium, European Molecular Biology Laboratory, Heidelberg, Jul 2023
- Signatures of Nonequilibrium Fluctuations in Life workshop, International Center for Theoretical Physics, Trieste, May 2023

Nonequilibrium design strategies for functional colloidal assemblies

- Autonomous Matter symposium, AMOLF, Amsterdam, April 2023
- Designing Soft Matter in and out of Equilibrium workshop, Leiden University, Leiden, Feb 2023
- Information in Matter symposium, AMOLF, Amsterdam, Nov 2022

Direct evaluation of rare events in active matter from variational path sampling

- Berkeley Statistical Mechanics Meeting, UC Berkeley, Jan 2022

Inverse design in trajectory space for nonequilibrium colloidal self-assembly

- Bay Area Theoretical Chemistry Poster Session, *virtual*, Jul 2021
- IOP Advanced School in Soft Condensed Matter, *virtual*, Jul 2021

Variational control forces for enhanced sampling of nonequilibrium molecular dynamics simulations

- Berkeley Statistical Mechanics Meeting, UC Berkeley, Jan 2020

Variational estimation of large deviation functions

- Northern California Theoretical Chemistry Meeting, UC Berkeley, May 2019
- Berkeley Statistical Mechanics Meeting, UC Berkeley, Jan 2019

Professional Service

Reviewing Service

- *Physical Review Letters*
- *Physical Review Research*
- *Nature Communications Physics*
- *Journal of Chemical Physics*
- *Journal of Statistical Mechanics: Theory and Experiment*
- *Reports on Progress in Physics*
- *Physica A: Statistical Mechanics and its Applications*

Mentorship

- Robin de Smit, Masters in Physics & Astronomy (Theoretical Physics track), University of Amsterdam, Sep 2024-Dec 2024
- Sofia Sauro, Masters in Physics & Astronomy (Biophysics and Biophotonics track), University of Amsterdam, Feb 2025-Aug 2025

Teaching Experience

University of California, Berkeley, CA

Founding Instructor **Summers 2020, 2021**

- UC Berkeley Math Bootcamp (Graduate Level)
  - As one of four instructors created a week-long math bootcamp for yearly ~ 50 physical chemistry PhD students.
  - Responsibilities included organizational work for logistics and funding, developing teaching material and practice problems and solutions on calculus, linear algebra, differential equations, probability and coding, instructional design in a bootcamp format, delivering lectures and leading discussion sections during the bootcamp.

Graduate Student Instructor **Fall 2017-Fall 2019**

- Thermodynamics and Statistical Mechanics (Graduate Level)
  - Sole teaching assistant for class of 48 students.
  - Responsibilities included holding biweekly office hours and weekly discussion sections, substitute lecturing and grading problem sets and exams.
- Advanced Quantum Mechanics (Graduate Level)
  - Sole teaching assistant for class of 29 students.
  - Responsibilities included holding biweekly office hours and weekly discussion sections, substitute lecturing, creating and grading problem sets and exams.
- General Chemistry (Undergraduate Level)
  - Sole laboratory instructor for two sections of 30 students each.
  - Responsibilities included conducting two 3h/week laboratory sections, grading lab reports and exams, and holding exam reviews and biweekly office hours.