# Nandan Haloi, PhD

Curriculum Vitae

# Education

- 2021 **Doctor of Philosophy in Biophysics and Quantitative Biology**, *University of Illinois at Urbana-Champaign*, Illinois, USA, PI: Emad Tajkhorshid.
- 2016 **Bachelors of Technology in Chemical Science and Technology**, *Indian Institute of Technology Guwahati*, Assam, India.

### Positions

- 2023–current **Marie-Curie Postdoctoral Fellow**, *KTH Royal Institute of Technology*, Stockholm, Sweden. Pl: Erik Lindahl
  - 2021–2023 **Postdoctoral Scholar**, *In Collaboration with Janssen Pharmaceutical*, Stockholm, Sweden. Pl: Erik Lindahl

### Research Expertise

Membrane Protein Function-Dynamics | Drug-Protein Interactions. Molecular Dynamics Simulations | Machine Learning | Integrative Modeling.

## Grants and Awards

Research

- 2023 Marie Skłodowska-Curie Actions (MSCA) Postdoctoral Fellowships (101107036). Characterizing ligand-protein interactions with a cryo-EM data-driven modeling approach
- 2022 EMBO Postdoctoral Fellowships Acknowledge of Excellence. Characterizing ligand-protein interactions with a cryo-EM data-driven modeling approach Supercomputing
- 2023 Main PI EuroHPC Regular Access Super-computing Grant (EHPC-REG-2023R01103), Investigating conformational modulation of neuronal receptors by brain neurosteroids (24 million CPU/GPU core hours).
- 2022 Main PI EuroHPC Regular Access Super-computing Grant (EHPC-REG-2021R0074), Characterizing conformational landscape of neuronal receptors (23 million CPU core hours).
- 2021 **Co-PI Illinois Blue Waters Super-computing Grant**, Mechanism of Antibiotic Resistance in Gram-negative Bacteria (estimated value of \$480K).

#### Travel and Others

- 2023 PRACE Travel Grant, International HPC Summer School.
- 2021 **Poster Competition Winner**, Biophysical Society Meeting.
- 2019 Biochemistry Travel Award, UIUC.
- 2019 Biophysics Travel Award, UIUC.

## Publications

#### Corresponding-author

- 2025 T. Shugaeva, R. J. Howard, **N. Haloi**<sup>†</sup>, and E. Lindahl<sup>†</sup>, "Modeling cryo-EM structures in alternative states with generative AI and density-guided simulations" <u>bioRxiv</u>, doi: https://doi.org/10.1101/2025.02.06.636862
- 2024 S. E. Lidbrink, R. J. Howard, N. Haloi<sup>†</sup>, and E. Lindahl<sup>†</sup>, "Resolving the conformational ensemble of a membrane protein by integrating small-angle scattering with AlphaFold" <u>bioRxiv</u>, doi: https://doi.org/10.1101/2024.09.05.611464

## First-author

- 2025 **N. Haloi,** R. J. Howard, and E. Lindahl, "Cryo-EM ligand building using generative AI and molecular dynamics "*bioRxiv*, doi: https://doi.org/10.1101/2025.02.10.637508
- 2025 N. Haloi, E. Karlsson, M. Delarue, R. J. Howard, E. Lindahl, "Discovering cryptic pocket opening and binding of a stimulant derivative in a vestibular site of the 5-HT<sub>3A</sub> receptor", <u>Science Advances</u>, 11, eadr0797.
- 2025 **N. Haloi**, S. E. Lidbrink, R. J. Howard, E. Lindahl, "Adaptive sampling-based structural prediction reveals opening of a GABA<sub>A</sub> receptor through the  $\alpha\beta$  interface" <u>Science Advances</u>, 11, eadq3788.
- 2024 N. Haloi\*, S. Huang\*, A. N. Nichols, E. J. Fine, C. B. Marotta, D. A. Dougherty, E. Lindahl, R. J. Howard, S. L. Mayo, H. A. Lester "Interactive computational and experimental approaches improve the sensitivity of periplasmic binding protein-based nicotine biosensors for measurements in biofluids" *Protein Engineering, Design and Selection*, 37, gzae003.
- 2022 A. K. Vasan\*, N. Haloi\*, P. C. Wen, R. J. Ulrich, M. E. Metcalf, W. W. Metcalf, P. Hergenrother, D. Shukla, and E. Tajkhorshid "Role of internal loop dynamics in antibiotic permeability of outer membrane porins" *PNAS*, 119(8):e2117009119.
- 2021 **N. Haloi\***, A. K. Vasan\*, E. Geddes, A. Prasanna, P. C. Wen, W. W. Metcalf, P. Hergenrother, and E. Tajkhorshid "Rationalizing generation of broad spectrum antibiotics with the addition of a positive charge" <u>*Chemical Science*</u>, 12:15028-15044. (2021) (Cover Article) (Featured at Illinois News Bureau and TCBG highlight)
- 2021 N. Haloi, P. C. Wen, Q. Cheng, M. Yang, G. Natarajan, A. K. S. Camara, W. M. Kwok, and E. Tajkhorshid "Structural basis of complex formation between mitochondrial anion channel VDAC1 and Hexokinase-II" *Communications Biology*, 4:667. (Featured at TACC's Stampede2 HPC Supercomputers, HPCwire newsletters and TCBG highlight)

### Co-author

- 2024 M. K. Kar, R. Mahata, S. Srimayee, N. Haloi, R. Kumar, E. Lindahl, M. Santra, and D. Manna, "β-Carboline-based light and pH dual stimuli-responsive ion transporters induce cancer cell death" <u>Chemical Communications</u>, 60, 8419.
- 2024 X. Yu\*, R. E. Matico\*, R. Miller, B. V. Schoubroeck, K. Grauwen, J. Suarez, B. Pietrak, N. Haloi, Y. Yin, G. Tresadern, L. Perez Benito, E. Lindahl, A. Bottelbergs, D. Oehlrich, N. V. Opdenbosch, S. Sharma "Cryo-EM structures of NLRP3 reveal its self-activation mechanism" *Nature Communications*, 15, 1164.
- 2023 J. Cowgill\*, C. Fan\*, N. Haloi, V. Tobiasson, Y. Zhuang, R. J. Howard, and E. Lindahl "Structure and dynamics of differential ligand binding in the human ρ-type GABAA receptor" <u>Neuron</u>, 111,1–15.
- 2023 V. Bondarenko, Q. Chen, K. Singewald, N. Haloi, T. Tillman, R. Howard, E. Lindahl, Y. Xu, P. Tang "Structural Elucidation of Ivermectin Binding to α7nAChR and the Induced Channel Desensitization" ACS Chemical Neuroscience 14, 6, 1156–1165

- 2023 S. Dey, A. Patel, N. Haloi, S. Srimayee, S. Paul, G. K. Barik, N. Akhtar, D. Shaw, G. Hazarika, B. M. Prusty, M. Kumar, M. K. Santra, E. Tajkhorshid, S. Bhattacharjee, D. Manna "Quinolinebased Zinc Ionophores with Antimicrobial Activity" *Journal of Medicinal Chemistry*, 66, 16, 11078–11093. (Cover Article)
- 2020 S. K. Bharathkar, B. W. Parker, A. Malyutin, **N. Haloi**, E. Tajkhorshid, and B. M. Stadtmueller "The structures of secretory and dimeric Immunoglobulin A" *eLife*, 9:e56098.
- 2020 J. T. Petroff, S. M. Omlid, N. Haloi, L. Sith, S. Johnson, and R. D. McCulla "Reactions of sulfenic acids with amines, thiols, and thiolates studied by quantum chemical calculations" *Computational and Theoretical Chemistry*, 1189: 112979.
- 2018 S. Gorai, D. Paul, R. Borah, N. Haloi, M. K. Santra, and D. Manna "Role of cationic groove and hydrophobic residues in Phosphatidylinositol-dependent membrane-binding properties of Tks5-Phox homology domain" *ChemistrySelect*, 3:1205-1214.
- 2016 S. Gorai, D. Paul, N. Haloi, R. Borah, M. K. Santra, and D. Manna "Mechanistic insights into the phosphatidylinositols binding properties of pleckstrin homology domain of lamellipodin" *Molecular BioSystems*, 12:747-57.

#### Teaching

- 2025 **Outreach Teaching**, Exploring Biomolecular Modeling and Simulations | Sabancı University, Istanbul.
- 2024 **Course Teaching**, Molecular Biophysics | Engineering Physics, KTH | Graduate.
- 2023 **Course Teaching**, Molecular Biophysics | Engineering Physics, KTH | Graduate.
- 2023 Outreach Teaching, Brain Awareness Week | High School, Stockholm.
- 2022 **Outreach Teaching**, Demonstrating the Power of Simulations | High School, Stockholm.
- 2021 **Course Teaching**, Cells, Tissues & Development | Department of Biochemistry, UIUC | Undergraduate.
- 2018 Course Teaching, Physical Biochemistry | Department of Biochemistry, UIUC | Undergraduate.

## Student Supervision

- 2024-2025 **Master's Student**, Elisei Mankov, *Stockholm University*. Improving cryo-EM resolution of ligands in protein-ligand complexes using deep learning
  - 2024 **Summer Internship Student**, Beatrice Pavesi, *University of Pavia*. Cryo-EM-guided machine learning to calculate free energy underlying protein conformational landscapes
- 2023-current **PhD Student**, Samuel Eriksson Lidbrink, *KTH Royal Institute of Technology*. Resolving the conformational ensemble of a membrane protein by integrating small-angle scattering with AlphaFold
- 2022-current **PhD Student**, Tatjana Shugaeva, *KTH Royal Institute of Technology*. Refining cryo-EM structures in alternative states through generative models and density-guided simulations

# Diversity, Equity, and Inclusion Activities

- 2024 Newcomer Mentor, Nema Problema, Sweden.
- 2023 Workshop Organizer, Understanding Cultural Differences, Campus Solna Biophysics Environment, Stockholm, Sweden.
- 2021 Seminar Moderator, Black in International Physics of Living Systems, UIUC, USA.
- 2021 Career Counselor, Gargaon College, Assam, India.
- 2019 Refugee Mentor, Foundation for International Medical Relief of Children, UIUC, USA.

# Scientific Services

#### **Board Member**

- 2024-current **Board Member of User Support Advisory Committee**, National Academic Infrastructure for Supercomputers, Sweden
  - 2017–2024 Member of Scientific Community, *Biophysical Society Meeting*. Reviewer
    - 2025 Grant Reviewer, IT4Innovations, HPC Center Czech Republic.
- 2022-current Scientific Article Reviewer, Nat. Commun., JCTC, and PLOS Comput. Biol..
  - 2019 Poster Competition Judge, Biophysical Society Meeting.

#### Organizer/Host

- 2023-current Organizer of MD/AI Biweekly Seminar, Molecular Biophysics Stockholm, Sweden.
  - 2023 Assistant Organizer of EBSA, Stockholm, Sweden.

## Conferences

#### Atomistic Model Refinement using Artificial Intelligence and Cryo-EM

- 2025 Machine Learning Applied to Macromolecular Structure and Function, USA. (Poster)
- 2024 Emerging Theoretical Approaches to Complement Single-Particle Cryo-Electron Microscopy, <u>Italy</u>. (Poster)

# Conformational Dynamics of Ligand-gated Ion Channels using Adaptive Sampling and Markov State Modeling

- 2024 Computational Chemistry Seminar at Technische Universität Berlin, Germany. (Talk)
- 2024 Structural Bioinformatics Seminar at Linköping University, Sweden. (Talk)
- 2024 Biophysical Society Meeting, Philadelphia, USA. (Poster)
- 2023 European Biophysical Societies Association, Stockholm, Sweden. (Talk)
- 2023 International HPC Summer School, Atlanta, USA. (Poster)

## Antibiotic Permeations through Porins in Gram-negative Bacteria using Enhanced Sampling Simulations

- 2022 1st Nordic Conference on Computational Chemistry, Gothenburg, Sweden. (Poster)
- 2022 Physical and Quantitative Approaches to Overcome Antibiotic Resistance BPS Thematic meeting, Stockholm, <u>Sweden</u>. (Talk)
- 2022 Protein Dynamics Conference, Aussios, France. (Poster)
- 2022 Molecular Graphics and Modelling Society, United Kingdom, Virtual. (Talk)
- 2021 Recent Advances in Modelling Rare Events (RARE2021), India, Virtual. (Poster)
- 2021 European Molecular Biology Organization, Virtual. (Talk)
- 2020 International Physics of Living Systems, Virtual. (Talk)
- 2018 Biophysical Society Meeting, San Francisco, California, USA. (Poster)
- 2018 Gordon Research Seminar, Ventura Beach, California, <u>USA</u>. (Talk) Complex Formation between VDAC and Hexokinase using Multi-scale Modeling

# 2020 Biophysical Society Meeting, San Diego, California, USA. (Poster)

2019 Biophysical Society Meeting, Baltimore, Maryland, USA. (Poster)

## On the news

- 2021 Scientists Discover how Antibiotics Penetrate Gram-negative Bacterial Cell Walls, Featured at research news of Illinois News Bureau, UIUC.
- 2021 TACC Supercomputer Delves into Protein Interactions, Featured at HPC Wire news letter.
- 2021 **Cell's Energy Secrets Revealed with Supercomputers**, *Press release at Texas Advanced Computing Center (TACC) news letter*.

# References

Email: wmkwok@mcw.edu Phone: +1 414-955-5683

• Prof. Erik Lindahl - Postdoc Mentor Professor of Biophysics, KTH Royal Institute of Technology Professor of Biophysics, Stockholm University Vice dean, Chemistry, Stockholm University co-Director, Swedish e-Science Research Center Chair, Chapter VII Royal Engineering Academy of Sciences Email: erik@kth.se Phone: +46-734618050 • Prof. Emad Tajkhorshid - PhD Supervisor Professor of Chemistry, Biophysics, Bioengineering, and Biophysics and Quantitative Biology Directory of NIH Center for Macromolecular Modeling and Bioinformatics Beckman Institute for Advanced Science and Technology University of Illinois at Urbana Champaign, IL, USA Email: emad@illinois.edu Phone: +1 217-244-6914 • Prof. Wai-Meng Kwok - Collaborator Professor of Anesthesiology, Pharmacology & Toxicology Cancer Center and Cardiovascular Center Medical College of Wisconsin, Milwaukee, WI, USA