

Sthitadhi Maiti

Websites: LinkedIn <https://www.linkedin.com/in/sthitadhimaiti>
Personal website: <https://smaiti7.github.io>

EDUCATION

- Doctor of Philosophy (Ph.D.)** in Chemistry, May 2024
School of Molecular Sciences,
Arizona State University, Tempe, Arizona, USA
CGPA: 3.76/4 (Overall)
Dissertation: Solvation Thermodynamics and Free Energy Surfaces of Intrinsically Disordered Proteins (IDPs) in Aqueous Solutions
- Master of Science (M.Sc.)** in Chemistry, 2014 – 2016
Department of Chemistry,
Indian Institute of Technology Guwahati, India
CGPA: 9.36/10 (Overall)
- Bachelor of Science (B.Sc.)** in Chemistry, 2011 – 2014
Department of Chemistry,
RKM Vidyamandira, Belur Math, University of Calcutta, India
CGPA: 7.1/10 (Overall)
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RESEARCH EXPERIENCE

Arizona State University

Ph.D. Research 2018 - 2024
Thesis: Solvation Thermodynamics and Free Energy Surfaces of Intrinsically Disordered Proteins (IDPs) in Aqueous Solutions.
Primary Advisor: Dr. Matthias Heyden

Skillset and experience

- Broad expertise in **classical Molecular Dynamics (MD) simulations of proteins with explicit water**, along with **steered MD**, and **umbrella sampling of IDPs** to estimate folding free energies from one state to another.
- Study the impact of **protein-water interactions** and empirical scaling parameters on the thermodynamics of protein solvation with explicit solvent classical MD simulations, using K-18 domain of Tau protein as the model system. ---- *JPC B. (Published Aug 9, 2023, <https://doi.org/10.1021/acs.jpcc.3c01726>)*
- Generate and analyze 3D maps of local contributions to the solvation free energy of intrinsically disordered proteins (programming in **Mathematica**, and **C**)
- Explore the feasibility to design peptide-based ligands with high binding affinity to **α -MoRF** (alpha-Molecular Recognition Feature) domains based on binding-induced folding mechanisms.
- Develop an automated simulation protocol for the calculation of peptide folding free energy profiles using simulation package of **GROMACS**, **PLUMED**, and **enhanced sampling** technique of **Umbrella Sampling**.
- Find **binding free energies** of antiapoptotic protein Mcl-1 to PUMA and other **α -MoRF**, BH3-only domains using **coarse grained umbrella sampling** in SIRAH forcefield, with an aim to study if the combined binding and folding free energies align with the experimentally observed binding free energies. ---- *Manuscript in prep.*
- Two **collaborative research works** with professors in Italy and at ASU resulting in two publications.

Ph.D. Research (previous) 2016 - 2018
Topic: Development of a Homogeneous Molybdenum Catalyst, and Synthesis of a Hypoxia Sensitive MRI Contrast Agent.

Advisor: Dr. Ryan Trovitch

Skillset and experience

- Designed, and performed, organometallic synthesis, and analyses such as IR, and NMR.
- Optimized separation/purification techniques -- column chromatography and crystallization of compounds.
- Performed organic synthesis of a modified Gd-DOTA MRI contrast agent to be used selectively in cells under hypoxic conditions. Used MALDI-TOF, and UV-Vis to analyze it.

Jawaharlal Nehru Center for Advanced Science and Research (JNCASR), Bangalore, India May-July 2015
Senior Summer Research Fellow (**Summer Internship**)

Project: Synthesis of Keggin Polyoxometalate Based Organic-Inorganic Hybrids for Applications in Catalysis and Biology. (Published in *Inorg. Chem.* in 2018)

Advisor: Dr. Sebastian C. Peter

Skillset and experience

- Developed and synthesized heterogeneous phosphomolybdates, and phosphotungstate catalysts using hydrothermal synthesis technique.
- Characterization using powder XRD, & SC-XRD (prepared the crystals for it)
- Analysis of oxidation products of organic conversions with GC-MS.
- Discovered small molecule oxidation property of the phosphotungstate catalysts on cyclooctene and ethyl benzene.

Indian Institute of Technology Guwahati, India (M.Sc.) 2014 - 2016

M.Sc. Research (Nov 2015- May 2016)

Thesis: A Novel Colorimetric and Fluorescence “Turn-On” Sensor for Hg(II) and Cu(II) ions.

Advisor: Dr. Gopal Das

Skillset and experience

- Designed, and synthesized organic ligands to bind to Hg(II) and Cu(II) ions.
- Analyzed them through IR, NMR and UV-vis study.
- Fluorescence study for Cu(II), and UV-Vis for colorimetric Hg(II) ion detection.

PUBLICATIONS

(5) **Maiti, S.**; Heyden, M. Prediction of Intrinsically Disordered α -MoRFs by examining Folding and Binding Free Energies. (*In preparation*)

(4) **Maiti, S.**; Heyden, M. Model-Dependent Solvation of the K-18 domain of the Intrinsically Disordered Protein Tau. *J. Phys. Chem. B.* **2023**, *127*, 33, 7220–7230.

(3) Nibali, V. C.; **Maiti, S.**; Saija, F.; Heyden, M.; Cassone, G. Electric-field induced entropic effects in liquid water. *J. Chem. Phys.* **2023**, *158*, 184501.

(2) Sauer, M.; Colburn, T.; **Maiti, S.**; Heyden, M.; Matyushov, D. Linear and Nonlinear Dielectric Response of Intrinsically Disordered Proteins. *J. Phys. Chem. Lett.* **2024**, *15*, 20, 5420–5427.

(1) Roy, S.; Vemuri, V.; **Maiti, S.**; Manoj, S. K.; Subbarao, U.; Peter, S. C. Two Keggin-based isostructural POMOF hybrids: synthesis, crystal structure, and catalytic properties. *Inorg. Chem.* **2018**, *57*, 19, 12078–12092.

TECHNICAL SKILLS AND PROFESSIONAL COURSES

Languages/Tech proficiency: Python, Wolfram Mathematica, C, Unix Shells (Bash), HPC, AWK, R, SQL and LaTeX.

Computational Chemistry Techniques: Molecular Dynamics, Enhanced Sampling (Umbrella Sampling, Metadynamics), Free-Energy Calculations, FEP, Protein-Ligand Docking, Virtual-screening, SAR analysis.

Computational Chemistry Packages: GROMACS, PLUMED, Rosetta, Schrodinger Maestro, and LiveDesign.

Molecule Visualization: Visual Molecular Dynamics (VMD), Chimera, PyMOL, and Avogadro.

Python Data Analysis & Machine Learning Packages/Frameworks: Pandas, Matplotlib, RDKit, scikit-learn, PyTorch, Tensorflow.

Other Software: Git, AutoDock Vina, Wavefunction Spartan, Chem Bio Draw, Blender, Adobe Illustrator, & Photoshop

Synthetic and Analytical Chem. Skills: Organic/Organometallic/Material Synthesis, Extraction & Purification, IR, NMR, UV-Vis, Fluorescence, MALDI, GC-MS, Powder XRD.

Online Courses: Schrödinger - 1. **Introduction to Molecular Modeling in Drug Discovery.**

<https://courses.schrodinger.com/certificates/jontoiwo1u>

2. **High-Throughput Virtual Screening for Hit Finding and Evaluation (HTVS).**

<https://courses.schrodinger.com/certificates/fr06qf4f3q>

Coursera - 1. **Supervised Machine Learning: Regression and Classification.**

<https://coursera.org/share/2d7c16350b79f5eccbb30f49eb32b16e>

TEACHING EXPERIENCE

2016(FALL): Graduate Teaching Assistant, CHM 113 Labs, General Chemistry

2017(SPR) – 2018(SPR): Graduate Teaching Assistant, CHM 116 Labs, General Chemistry

2018(SUMMER): Graduate Teaching Assistant, CHM 116 Labs, General Chemistry

2018(FALL) – 2019(SPR): Graduate Teaching Assistant, CHM 116 Labs, General Chemistry

2021(FALL) – 2024(SPR): Graduate Teaching Assistant, BCH 341 & CHM 114 OL, Biochemistry & Chemistry

CHM 113, 116: General Chemistry Labs with 25 students per lab. Taught 4 different batches of students per week.

BCH 341: Physical Chem with Bio Focus. About 150 students per semester. Had to interact one-on-one during weekly office hours and revision days.

CHM 114 OL: Online lab for General Chemistry for Engineers with about 60 students per TA. Had to grade reports, homework, and answer questions online.

PRESENTATIONS

ACS Fall 2023, San Francisco (2023): Maiti, S.; Heyden, M*. Solvation Thermodynamics and Free Energy Profiles of Intrinsically Disordered Peptides and Alpha-MoRFs (POSTER).

ACS Spring 2023, Indianapolis (2023): Maiti, S.; Heyden, M*. Alpha-MoRF and Folding Free Energy Prediction in Intrinsically Disordered Peptides (POSTER).

Biophysical Society (BPS), San Diego (2023): Maiti, S.; Heyden, M*. Prediction of Alpha-MoRF and Folding Free Energies in Intrinsically Disordered Peptides (POSTER).

Les Houches-TSRC Workshop on Protein Dynamics, Aussois, France (2022): Maiti, S.; Heyden, M*. Free Energy Surface Contributions for Intrinsically Disordered Proteins in Atomistic Simulations (POSTER).

ACS Fall 2019, San Diego (2019): Maiti, S.; Heyden, M*. Solvation Thermodynamics of Intrinsically Disordered Proteins (POSTER).

AWARDS & HONORS

Secured an **All-India-Rank of 91** in **IIT-JAM Joint Admission Entrance Exam** for M.Sc. (among around **6000** candidates).

Awarded the **Innovation in Science Pursuit for Inspired Research (INSPIRE)** Fellowship by Department of Science and Technology, Government of India from 2011-2016 for undergraduate and masters studies. It's granted to the top 1% of students in India based on merit/scores.

Secured an **All-India-Rank of 25 out of 755** selected Lectureship candidates in the National Eligibility Test (NET), Chemical Science (among around **50,000** candidates).

Awarded the **JBNSTS (Jagadish Bose National Science Talent Search) 2011 Senior Scholarship** — one of the most prestigious academic awards in West Bengal, and India (Among selected **56 undergraduate students out of 2000 applicants**)

Selected for internship under **SRFP (Summer Research Fellowship Program) 2015** at **JNCASR (Jawaharlal Nehru Centre for Advanced Scientific Research), Bangalore** under **Dr. Sebastian C. Peter**. About 150 fellowships are offered out of around 2000 applications each year during the summer months from May to July end.

VOLUNTEERING & EXTRA-CURRICULAR ACTIVITIES

Signed up as one of the **Grand Award Judges (Chemistry) for Intel Science and Engineering Fair (ISEF) 2019, Phoenix**, under Society for Science & the Public on May 14th & 15th 2019.

On Sept 2018, under the **National Speleological Society**, volunteered for **Peppersauce caves graffiti removal and restoration project** in a team of 6-7 ASU students, and several Central Arizona Grotto members. [Peppersauce cave restoration report Sept 21-23, 2018](#)

As a member of the **Outreach Choir at ASU**, offered services as one of the choir singers among a group that visited retirement homes around Phoenix area on the weekends (thrice a semester) and sing for the people there. (Aug 2018 – Mar 2020)

Chief of Safety, Amateur Radio Club at ASU (W7ASU). Undertaken operational safety during club activities at one of the oldest Ham Radio clubs at the Arizona State University, from Aug 2022 – Dec 2023.

Designed **the club logo of W7ASU**, taking inspiration from the previous logo, and combining own ideas.
