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Sthitadhi Maiti

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EDUCATION

Doctor of Philosophy (Ph.D.) in Chemistry, Aug 2016 – 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)

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 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.jpcb.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 (**α**-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 enhance 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.*

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, XXX, 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: Python, Wolfram Mathematica, C, Unix Shells (Bash), AWK, R 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.
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.
Schrodinger Online Courses:
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

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.