Sthitadhi Maiti

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EDUCATION

PhD in Chemistry, May 2024

School of Molecular Sciences, Arizona State University, Tempe AZ (CGPA: 3.76)

Master of Science in Chemistry, May 2016

Indian Institute of Technology Guwahati, India

Bachelor of Science in Chemistry, May 2014

Ramakrishna Mission Vidyamandira, Belur Math, India

TECHNICAL SKILLS & INTERESTS

Technical Skills: ***Chemistry/Biophysics/Statistics***- Research | Computational Chemistry | Biochemistry | Classical Molecular Dynamics | Enhanced Sampling | Umbrella sampling | Free Energy Calculations | FEP | Statistical Data Analysis | Drug design | Structure & Ligand Based Virtual Screening | Docking | Shape Screening | R-group Enumeration.

Programming/Software- Wolfram Mathematica | GROMACS | VMD | PyMOL | Chimera | Schrodinger Maestro | LiveDesign | Bash scripting | Python | C | Linux | HPC | Rosetta | PyRosetta | Wavefunction Spartan | Modeller | AutoDock Vina | Pandas | Matplotlib | Machine Learning | RDKit | scikit-learn | PyTorch | R | Blender | CSS | LaTeX | ChemDraw | Excel.

Experimental- Organometallic/Material Synthesis | Extraction and Purification | IR | UV-Vis | Fluorescence | NMR | GC-MS | Powder XRD.

Communication Skills: Teaching assistant in undergraduate chemistry labs (Gen Chem 113, 116) for six semesters.

Interests: Reading popular science articles | Graphic Designing on Photoshop, Illustrator & Blender | Photography | Hiking

RESEARCH EXPERIENCE

Research Assistant at Dr. Matthias Heyden's Computational Chemistry Lab, ASU (08/2018 – present)

- 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 disordered Tau protein as the model system.
  ---- *J. Phys. Chem. B.* **2023**, 127, 33, 7220–7230.
- 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 domains using **coarse grained umbrella sampling** in SIRAH forcefield, with an aim to correlate them with the folding free energy penalties of the BH3 domains.
  ---- *Manuscript in prep.*

Research Assistant at Dr. Ryan Trovitch's Organometallic Synthesis Lab, ASU (07/2016 – 08/2018)

- 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.

Research Intern at Dr. Sebastian C. Peter's Solid State & Inorganic Chemistry Lab, JNCASR, India (05/2015 – 07/2015)

- Developed, synthesized, and characterized (with powder XRD & SC-XRD) heterogeneous phosphomolybdates, and phosphotungstate catalysts for small molecule oxidation. Published in Inorganic Chemistry in 2018.

Research Intern (M.Sc.) at Dr. Gopal Das' Supramolecular Chemistry Lab, IIT Guwahati, India (11/2015 – 05/2016)

- Developed, synthesized, and characterized (with UV-vis, IR and NMR) a colorimetric and fluorescence "Turn-On"sensor for the detection of Hg(II) and Cu(II) ions.

EXTRACURRICULAR EXPERIENCE AND AWARDS

- Judged high school students' science experiments as a Grand Award Judge (Chemistry) for Intel Science and Engineering Fair 2019, May 14-15, Phoenix, AZ.
- Manage the Amateur Radio Club at ASU (W7ASU) as one of its current officers and designed the current logo of W7ASU.
- Attended weekly meetings of Machine Learning Club, Sun Devil Data Science, Linux Users Group, Code Devils and SoDA at ASU.
- Awarded the JBNSTS (Jagadish Bose National Science Talent Search) 2011 Senior Scholarship & DST Inspire Fellowship, Govt. Of India for the period of 2011-2016.

ACADEMIC CONFERENCES AND WORKSHOPS

- Attended and presented a poster at the ACS Fall 2019 Conference in San Diego on Solvation Thermodynamics of Intrinsically Disordered Proteins (IDPs).
- Presented poster at the Les Houches Protein Dynamics Workshop at Aussois, France, in 2022 on Free Energy Surface Contribution for IDPs in Atomistic Simulations.
- Research poster presentation at Biophysical Society 2023 Feb 18-22 in San Diego.
- Poster presentation at ACS Spring 2023 in Indianapolis, and at ACS Fall 2023, San Francisco.
- Attended workshops, "Python for Data Science in Chemistry," at ACS Spring and Fall 2023.
- Schrodinger Online Courses: 1. **Introduction to Molecular Modeling in Drug Discovery**. (Completed 11/15/2023) https://courses.schrodinger.com/certificates/jontoiwo1u
  2. **High-Throughput Virtual Screening for Hit Finding and Evaluation**. (Completed 02/27/2024) https://courses.schrodinger.com/certificates/fr06qf4f3q

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**.; Matyushov, D. Linear and Nonlinear Dielectric Response of Intrinsically Disordered Proteins. (*Submitted to JPCL on Mar 22*)

(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.