DAIPAYAN SARKAR

Molecular Dynamics | Computational Biophysics | Thermodynamics | Chemical Kinetics | Free-Energy Methods | Enhanced Sampling | Cryo-EM

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EXPERIENCE

Postdoctoral Research Scientist

MSU-DOE Plant Research Laboratory

May 2021 – | East Lansing, MI

- Multi-million atom molecular dynamics (MD) simulations at atomic resolution to quantify the permeabilty of small photosynthetic metabolites across bacterial microcompartment shells found in photosynthetic cyanobacteria.
- Membrane permeability calculations using enhanced sampling method - Replica Exchange Umbrella Sampling (REUS).
- Membrane protein simulations and Free Energy Perturbation (FEP) to find the change in the free energy of binding ($\Delta G_{binding}$) for small compounds.
- Data-guided integrative modeling (using experimental methods such as Cryo-EM, NMR)

Postdoctoral Research Associate

Department of Biological Sciences, Purdue University

July 2019 – Apr 2021 | West Lafayette, IN

- Using shape complementarity algorithm for protein-protein interactions, specifically for membrane proteins, for the challenge of CAPRI protein binding.
- Protein structure refinement using molecular dynamics and enhanced sampling (Gaussian Accerelated MD, Metadynamics) to improve the quality of predicted structures, predicted using a deep learning-based algorithm in the CASP14.
- Cryo-EM protein structure refinement and ligand challenge to flexibly fit protein structures and ligand in EM density maps for EMChallenge2021.
- Quantifying protein (OCRL1) conformational change and quantify lipid interactions due to mutations occurring in Lowe syndrome.

Postdoctoral Research Associate

Department of Mechanical Engineering, University of Texas, Dallas

June 2017 – June 2019 | Richardson, TX

- A chemical kinetic (reaction- diffusion) model was used to determine the rate of temperature-dependent plasmonic protein inactivation. The concept developed has been extended to major applications in areas of targeted drug delivery and diffusion across the blood-brain barrier.

Adjunct Lecturer

Department of Mechanical Engineering, University of Texas, Arlington

Jan 2017 – May 2017 | Arlington, TX

- Taught the undergraduate course in the fundamentals of thermodynamics, chemical kinetics, and heat transfer.

SOFTWARE SKILLS

Molecular Dynamics - NAMD, GROMACS, VMD
Free Energy calculations (REUS, ABF), FEP
Enhanced sampling (GAMD, Metadynamics)
QM - Single point energy, Optimization (Gaussian16)
Python, Tcl, Bash, MATLAB
Docking: Autodock-Vina, RosettaDock, HADDOCK

HIGHLIGHTS

Cryo-EM structure of AztraZeneca COVID-19 viral vector, ChAdOx1 (PDB: 7RD1)
We used molecular dynamics and cryo-EM density to flexibly fit protein subunits into the density map. Using state-of-the-art molecular simulations and SPR experiments, the data confirmed that the PF4 protein is capable of forming stable complexes with clinically relevant adenoviruses, an important step in unraveling the mechanisms underlying the thrombocytopenia syndrome. This work was published in Science Advances and was highlighted worldwide in media platforms such as BBC, EurekAlert (AAAS), to name a few.

ISPR-DOE award for 18th International Photosynthesis Congress in Dunedin, New Zealand
This award was awarded to present my current research on the transport of photosynthetic metabolites (or substrates) across bacterial microcompartments. This research aims at providing a mechanistic view of the permeability of small molecules across microcompartments and determining the rate-limiting step of the transport of these photosynthetic compounds. Research can be applied to sustainable, metabolic and bioengineering applications.

Doctoral Dissertation Fellowship
Awarded annually by College of Engineering, University of Texas at Arlington, to select PhD students for outstanding research.

STRENGTHS

Hard-working
Fast-learner
Research, Creativity & Problem Solving
Self-motivated & Leader
Teamwork & Mentorship
Communication Skills
Technical Writing & Presentations

EDUCATION

Ph.D. Mechanical Engineering

University of Texas, Arlington, USA

Aug 2012 – Aug 2016

M.S. Mechanical Engineering

University of Texas, Arlington, USA

Aug 2010 – May 2012

B.Eng. Mechanical Engineering

University of Mumbai, India

May 2006 – May 2010

Structure prediction: BLAST, Modeller, AlphaFold
ROSETTA, UCSF Chimera, Phenix
Linux, HPC (Slurm, Torque)

SELECTED PUBLICATIONS

Journal Articles

- Gupta, C., Sarkar, D., Tieleman, D. P., & Singharoy, A. (2022). The ugly, bad, and good stories of large-scale biomolecular simulations. *Current Opinion in Structural Biology*, *73*, 102338. doi:10.1016/j.sbi.2022.102338
- Vant, J. W., Sarkar, D., Nguyen, J., Baker, A. T., Vermaas, J. V., & Singharoy, A. (2022). Exploring cryo-electron microscopy with molecular dynamics. *Biochemical Society Transactions*, *50*(1), 569–581. doi:10.1042/BST20210485
- Baker, A. T., Boyd, R. J., Sarkar, D., Teijeira-Crespo, A., Chan, C. K., … Borad, M. J. (2021). ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome. *Science Advances*, *7*(49), eabl8213. doi:10.1126/sciadv.abl8213
- Lawson, C. L., Kryshtafovych, A., Adams, P. D., Afonine, P. V., Baker, M. L., … Chiu, W. (2021). Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. *Nature Methods*, *18*(2), 156–164. doi:10.1038/s41592-020-01051-w
- Lensink, M. F., Brysbaert, G., Mauri, T., Nadzirin, N., Velankar, S., … Wodak, S. J. (2021). Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function, and Bioinformatics*, *89*(12), 1800–1823. doi:10.1002/prot.26222
- Shekhar, M., Terashi, G., Gupta, C., Sarkar, D., Debussche, G., … Singharoy, A. (2021). CryoFold: Determining protein structures and data-guided ensembles from cryo-EM density maps. *Matter*, *4*(10), 3195–3216. doi:10.1016/j.matt.2021.09.004
- Aderinwale, T., Christoffer, C. W., Sarkar, D., Alnabati, E., & Kihara, D. (2020). Computational structure modeling for diverse categories of macromolecular interactions. *Current Opinion in Structural Biology*, *64*, 1–8. doi:10.1016/j.sbi.2020.05.017
- Vant, J. W., Lahey, S.-L. J., Jana, K., Shekhar, M., Sarkar, D., … Singharoy, A. (2020). Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. *Journal of Chemical Information and Modeling*, *60*(5), 2591–2604. doi:10.1021/acs.jcim.9b01167
- Vant, J. W., Sarkar, D., Streitwieser, E., Fiorin, G., Skeel, R., … Singharoy, A. (2020). Data-guided Multi-Map variables for ensemble refinement of molecular movies. *The Journal of Chemical Physics*, *153*(21), 214102. doi:10.1063/5.0022433
- Sarkar, D., Kang, P., Nielsen, S. O., & Qin, Z. (2019). Non-Arrhenius Reaction-Diffusion Kinetics for Protein Inactivation over a Large Temperature Range. *ACS Nano*, *13*(8), 8669–8679. doi:10.1021/acsnano.9b00068
- Sarkar, D., Haji-Sheikh, A., & Jain, A. (2015). Temperature distribution in multi-layer skin tissue in presence of a tumor. *International Journal of Heat and Mass Transfer*, *91*, 602–610. doi:10.1016/j.ijheatmasstransfer.2015.07.089

Conference Proceedings

- Doole, F. T., Chan, C. K., Streitwieser, E., Sarkar, D., Struts, A. V., … Brown, M. F. (2022). Rivalry of cholesterol and antimicrobial peptides as seen by molecular simulations and NMR spectroscopy. In *Biophysical Journal* (Vol. 121, 161a–162a). doi:10.1016/j.bpj.2021.11.1922
- Sarkar, D., Egelston, J. L., & Vermaas, J. V. (2022). Correlating the transport cycle of small multidrug resistance transporters. In *Biophysical Journal* (Vol. 121, 393a–394a). doi:10.1016/j.bpj.2021.11.800
- Doole, F. T., Chan, C. K., Streitwieser, E., Sarkar, D., Kim, M., … Brown, M. F. (2021). Antimicrobial Peptide-Membrane Interactions: Insights from Molecular Simulations. In *Biophysical Journal* (Vol. 120, 141a). doi:10.1016/j.bpj.2020.11.1052

Pre-prints

- Sarkar, D., Santiago, I., & Vermaas, J. (2022). Atomistic Origins of Biomass Recalcitrance in Organosolv Pretreatment. doi:10.26434/chemrxiv-2022-9j7zv
- Sarkar, D., Lee, H., Vant, J. W., Turilli, M., Jha, S., & Singharoy, A. (2021). Scalable Adaptive Protein Ensemble Refinement Integrating Flexible Fitting. doi:10.1101/2021.12.07.471672

*For a complete record of all publications, refer to my google scholar on page 1.

REFEREES

Dr. Josh Vermaas
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Association: Scientific collaborator (since 2017) and supervisor for AstraZeneca COVID-19 vaccine work.

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SYNERGISTIC SCIENCE