

# DAIPAYAN SARKAR

Biophysics | Thermodynamics and Kinetics | Cryo-EM | Reaction-Diffusion Models | Molecular Dynamics | Finite Element Methods

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## EXPERIENCE

### Postdoctoral Research Scientist

MSU-DOE Plant Research Laboratory, Michigan State University

May 2021 – Ongoing East Lansing, MI

- Using molecular dynamics simulations, we are collaborating with our experimental colleagues to improve photosynthetic yield and contribute towards building a sustainable bio-economy. We do so by providing mechanistic view - thermodynamics (free-energy) and kinetics (mean passage time) for transport of small photosynthetic molecules in cyanobacteria and C3/C4 plants.

### 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 CAPRI protein docking challenge.
- Protein structure refinement using molecular dynamics and enhanced sampling for structures predicted using deep learning based algorithm in CASP14 protein structure prediction challenge.
- 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

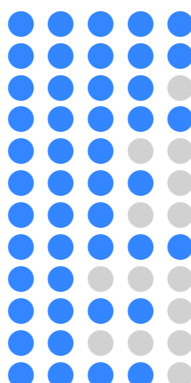
Department of Mechanical Engineering, University of Texas, Arlington

Jan 2017 – May 2017 Arlington, TX

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

## SOFTWARE SKILLS

Molecular Dynamics - NAMD, GROMACS  
VMD, VMD-Python  
Tcl, Bash  
Python, MATLAB for ODE/PDE solvers  
Autodock-Vina, MOE  
COMSOL Multiphysics (FEM)  
SOLIDWORKS (CAD)  
Linux, HPC (Slurm, Torque)  
C++, Scikit-Learn  
BLAST, HHPred, Modeller, AlphaFold  
ROSETTA, Pymol, UCSF Chimera, Phenix  
LaTeX



## 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 sub-units into the density map. Using state-of-the-art molecular simulations and SPR experiments, the data confirmed that PF4 protein is capable of forming stable complexes with clinically relevant Adenoviruses, an important step in unraveling the mechanisms underlying 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 towards presenting my current research on transport of photosynthetic metabolites (or substrates) across bacterial microcompartments. This research aims at providing a mechanistic view behind permeability of small molecules across microcompartments and determining the rate limiting step of the transport of these photosynthetic compounds. The research can be applied to sustainable, metabolic and bio-engineering 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

## RELEVANT PUBLICATIONS

### Books

- Wilson, E., Vant, J., Layton, J., Boyd, R., Lee, H., Turilli, M., Hernández, B., Wilkinson, S., Jha, S., Gupta, C., Sarkar, D., & Singharoy, A. (2021). *Large-Scale Molecular Dynamics Simulations of Cellular Compartments* (J. Schmidt-Krey, I.; Gumbart, Ed.). doi:10.1007/978-1-0716-1394-8\_18

### 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
- Baker, A. T., Boyd, R. J., Sarkar, D., Teixeira-Crespo, A., Chan, C. K., Bates, E., Waraich, K., Vant, J., Wilson, E., Truong, C. D., Lipka-Lloyd, M., ... Borad, M. J. (2021). ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome. *Science Advances*, 7(49). doi:10.1126/sciadv.abl8213
- Ramadesikan, S., Skiba, L., Lee, J., Madhivanan, K., Sarkar, D., De La Fuente, A., Hanna, C. B., Terashi, G., Hazbun, T., Kihara, D., & Aguilar, R. C. (2021). Genotype & phenotype in Lowe Syndrome: specific OCRL1 patient mutations differentially impact cellular phenotypes. *Human Molecular Genetics*, 30(3-4), 198-212. doi:10.1093/hmg/ddab025
- Sarkar, D., Lee, H., Vant, J. W., Trulli, M., Jha, S., & Singharoy, A. (2021). Scalable Adaptive Protein Ensemble Refinement Integrating Flexible Fitting. *bioRxiv : the preprint server for biology*. doi:10.1101/2021.12.07.471672
- Vant, J. W., Lahey, S.-L. J., Jana, K., Shekhar, M., Sarkar, D., Munk, B. H., Kleinekathöfer, U., Mittal, S., Rowley, C., & 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., Vermaas, J. V., & 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/acs.nano.9b00068
- Sarkar, D., Haji-Sheikh, A., & Jain, A. (2015a). 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., Kit Chan, C., Streitwieser, E., Sarkar, D., Struts, A. V., Singharoy, A., & Brown, M. F. (2022). Rivalry of cholesterol and antimicrobial peptides as seen by molecular simulations and NMR spectroscopy. (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. (Vol. 121, 393a-394a). doi:10.1016/j.bpj.2021.11.800
- Sarkar, D., Haji-Sheikh, A., & Jain, A. (2015b). Theoretical Analysis of Transient Bioheat Transfer in Multi-Layer Tissue. In *Volume 3: Biomedical and biotechnology engineering*. doi:10.1115/IMECE2015-53392
- Sarkar, D., Jain, A., & Haji-Sheikh, A. (2013). Analytical Temperature Distribution in a Multi-Layer Tissue Structure in the Presence of a Tumor. In *Volume 8a: Heat transfer and thermal engineering*. doi:10.1115/IMECE2013-63275

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

## REFEREES

### Prof. Josh Vermaas

@ Michigan State University

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Assistant Professor  
MSU-DOE Plant Research Laboratory  
1130 Molecular Plant Sciences  
East Lansing, MI 48824  
Association: Postdoc Advisor

### Prof. Abhishek Singharoy

@ Arizona State University

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Assistant Professor  
School of Molecular Sciences  
Tempe, AZ 85287-1604  
Association: Scientific collaborator (since 2017) and supervisor for AstraZeneca COVID-19 vaccine work.

### Prof. Ankur Jain

@ The University of Texas at Arlington

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Associate Professor  
Department of Mechanical and Aerospace Engineering, Bioengineering (affiliated)  
500 W 1st St  
Arlington, TX 76010  
Association: Ph.D. supervisor