

DAIPAYAN SARKAR



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SUMMARY

My research is in understanding the principles that govern energy conversion and storage in biological systems, such as in plants and cyanobacteria. The research is part of a DOE institutional goal, to improve photosynthetic yield and contribute towards building a sustainable bio-economy. In my research, I use computational methods such as molecular dynamics to determine thermodynamics (free-energy) of states and kinetics (mean passage time) between thermodynamic states, to understand the physical, chemical and mechanical properties of biological systems. The goal of my research is to develop high fidelity physics based and data-integrated multiscale models, in collaboration with experimental colleagues, to study photosynthetic systems to deliver renewable energy and sustainable bioproducts.

Technical Skills:

Molecular Dynamics Software: NAMD, GROMACS, VMD, VMD-Python

Programming: Python, C++, Tcl, Bash, MATLAB, Mathematica

Bioinformatics: AlphaFold, BLAST, HHPred, ROSETTA, Pymol, AutoDock Vina

Structural Biology: Phenix, MolProbity, UCSF Chimera.

Finite Element Analysis: COMSOL, ANSYS

Data Analysis: Python, MATLAB, Mathematica, OriginLab, Excel

High performance computing (HPC): Slurm, Torque

Operating system: Unix, MacOS, Windows

Utility: Microsoft Office, LaTeX

ACADEMIC PREPARATION

Postdoctoral Research Associate (PI: Dr. Josh V. Vermaas), MSU-DOE Plant Research Laboratory, Michigan State University, East Lansing, MI 48824, May 2021 -

Postdoctoral Research Associate (PI: Dr. Diasuke Kihara), Department of Biological Sciences, Purdue University, West Lafayette, IN, USA, July 2019 - April 2021

Postdoctoral Research Associate (PI: Dr. Zhenpeng Qin), Department of Mechanical Engineering, University of Texas at Dallas, Richardson, TX, USA, June 2017 - June 2019

Adjunct Lecturer, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, January 2017 - May 2017

Enhanced Graduate Teaching Assistant, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, August 2015 - May 2016

Summer Research Fellow (PI: Prof. Vinod Srinivasan (now at University of Minnesota, Twin Cities)), Department of Mechanical Engineering, Indian Institute of Science, Bengaluru, India, May 2015 - August 2015

Graduate Teaching Assistant, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, August 2012 - May 2015

Graduate Researcher, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, August 2010 - May 2012

Courtesy Affiliation (PI: Dr. Abhishek Singharoy), School of Molecular Sciences, Arizona State University, Tempe, AZ, USA, August 2018 -

EDUCATION

University of Texas at Arlington	August 2012 - August 2016
PhD , Mechanical Engineering	
University of Texas at Arlington	August 2010 - May 2012
MS , Mechanical Engineering	
University of Mumbai	May 2006 - May 2010
B. Eng. , Mechanical Engineering	

SERVICE

Review editor for Frontiers in Molecular Biosciences and Frontiers in Applied Mathematics and Statistics

Review editor for IEEE Transactions on Components, Packaging and Manufacturing Technology

Judge for undergraduate and graduate research competition, College of Engineering, UT-Arlington, 2021.

PEER-REVIEWED PUBLICATIONS

(* - joint first author contribution, ** - joint second author contribution)

1. C. Gupta, **D. Sarkar**, D. P. Tieleman, A. Singharoy, The ugly, bad, and good stories of large-scale biomolecular simulations, *Current Opinion in Structural Biology*, 2002, 73, 102338
2. J.W. Vant, **D. Sarkar**, J. Nguyen, A. T. Baker, J. V. Vermaas, A Singharoy, Exploring cryo-electron microscopy with molecular dynamics, *Biochemical Society Transactions*, 50 (1), 2022, 569-581.
3. A. T. Baker*, R. J. Boyd*, **D. Sarkar****, A. Teijeira-Crespo**, C. K. Chan**, E. A. Bates, K. Waraich, J.W. Vant, E.A. Wilson, C. D. Truong, M. Lipka-Lloyd, Petra Fromme, Josh V. Vermaas, D. Williams, L. Machiesky, M. Heurich, B. Nagalo, L. Coughlan, S. Umlauf, P. Chiu, P.J. Rizkallah, A.L.Parker, A. Singharoy, M. J. Borad, ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome, *Science Advances*, 2021, doi: 10.1126/sciadv.abl8213
4. M. Shekhar, G. Terashi, C. Gupta, **D. Sarkar**, G. Debussche, N. J. Sisco, J. Nguyen, A. Mondal, J. Vant, P. Fromme, W. D. Van Horn, E. Tajkhorshid, D. Kihara, K. Dill, A. Perez, A. Singharoy, 2021, *Matter*, Cell Press, 2021, doi:10.1016/j.matt.2021.09.004
5. A. Kryshtafovych, J. Moulton, ..., AlphaFold team ... **D. Sarkar** ..., Modeling SARS-CoV-2 proteins in the CASP-commons experiment, *Proteins*, 2021, 89(12): 1987- 1996, doi:10.1002/prot.26231
6. M. Lensink, ..., C. Christoffer, G. Terashi, J. Verburt, **D. Sarkar**, T Aderinwale, X Wang, D Kihara, ..., Shoshana J. Wodak, Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment, 2021, *Proteins: Structure, Function, and Bioinformatics*, doi:10.1002/prot.26222.

7. C.L. Lawson, A. Kryshchuk, P.D. Adams, P. Afonine, M. L. Baker, B. A. Barad, P. Bond, T. Burnley, R. Cao, J. Cheng, G. Chojnowski, K. Cowtan, K. A. Dill, F. DiMaio, D. Farrell, J. S. Fraser, M. A. Herzik, S. W. Hoh, J. Hou, L. Hung, M. Igaev, A. P. Joseph, D. Kihara, D. Kumar, S. Mittal, B. Monastyrskyy, M. Olek, C. Palmer, A. Patwardhan, A. Perez, J. Pfab, G. D. Pintilie, J. S. Richardson, P. B. Rosenthal, **D. Sarkar**, L. U. Schaefer, M. F. Schmid, G. F. Schroeder, M. Shekhar, D. Si, A. Singharoy, G. Terashi, T. C. Terwilliger, A. Vaiana, L. Wang, Z. Wang, S. A. Wankowicz, C. J. Williams, M. Winn, T. Wu, X. Yu, K. Zhang, H. M. Berman, W. Chiu, Outcomes of the 2019 EMDDataResource model challenge: validation of cryo-EM models at near-atomic resolution, 2021, *Nature Methods*, 18, 156 - 164.
8. S. Ramadesikan, L. Skiba, J. Lee, K. Madhivanan, **D. Sarkar**, A. De La Fuente, C. B. Hanna, T. Hazbun, D. Kihara, R. C. Aguilar, Specific OCRL1 patient mutations differentially impact Lowe Syndrome cellular phenotypes, 2021, *Human Molecular Genetics*, ddab025
9. T. Aderinwale, C. W. Christoffer, **D. Sarkar**, E. Alnabati, D. Kihara, Computational structure modeling for diverse categories of macromolecular interactions, 2020, *Current Opinion in Structural Biology*, 64, 1-8.
10. J. W. Vant, **D. Sarkar**, E. Strietweiser, G. Fiorin, R. D. Skeel, J. V. Vermaas, A. Singharoy, Data-guided Multi-Map variables for ensemble refinement of molecular movies, 2020, *Journal of Chemical Physics*, 153, 214102.
11. J.W. Vant, S. J. Lahey, K. Jana, M. Shekhar, **D. Sarkar**, B. H. Munk, U. Kleinekathofer, S. Mittal, C. Rowley, A. Singharoy, Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials, 2020, *Journal of Chemical Information and Modeling*, 60, 5, 2591–2604.
12. **D. Sarkar***, P. Kang*, S.O. Nielsen, Z. Qin, Non-Arrhenius Reaction-Diffusion Kinetics for Protein Unfolding over a Large Temperature Range, 2019, *ACS Nano*, 13, 8, 8669-8679.
13. S. Luhar, **D. Sarkar**, A. Jain, Steady state and transient analytical modelling of non-uniform convective cooling of a microprocessor chip due to jet impingement, 2017, *Int. J. Heat and Mass Transfer*, 110, 768-777 2017.
14. D. Anthony, **D. Sarkar**, A. Jain, Non-invasive, transient measurement of the core temperature of a solid body, 2016, *Scientific Reports*, 6, 35886:1-1.
15. D. Anthony, **D. Sarkar**, A. Jain, Contactless, non-intrusive core temperature measurement of a solid body in steady-state, 2016, *Int. J. Heat and Mass Transfer*, 101, 779-788.
16. **D. Sarkar**, A. Jain, R. J. Goldstein, V. Srinivasan, Corrections for lateral conduction error in steady-state heat transfer measurements, 2016, *Int. J. of Thermal Sciences*, 109, 413-423.
17. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Thermal conduction in an orthotropic sphere with spatial variation in convective heat transfer coefficient, 2016, *Int. J. Heat and Mass Transfer*, 96, 406-412.
18. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Steady-state temperature distribution in tissue due to heat generating tumor, 2015, *Int. J. Heat and Mass Transfer*, 96, 406-412.
19. **D. Sarkar**, K. Shah, A. Haji-Sheikh, A. Jain, Analytical modelling of temperature distribution in an anisotropic cylinder with circumferentially-varying convective heat transfer, 2014, *Int. J. Heat and Mass Transfer*, 39, 1027-1033.

20. **D. Sarkar**, A. Haji-Sheikh, A view of thermal wave in thin plates, 2012, *Communications in Heat and Mass Transfer*, 39, 8, 1009-1017.

Book Chapters

1. J. W. Vant*, **D. Sarkar***, C. Gupta*, M. Shekhar, S. Mittal and A. Singharoy, Molecular Dynamics Flexible Fitting: All you want to know about flexible fitting, *Methods in Molecular Biology, Protein Structure Prediction*, 4th Ed - in press, 2019 (role: equal contribution)
2. E. Wilson, J. W. Vant, J. Layton, R. Boyd, H. Lee, M. Turilli, B. Hernandez, S. Wilkinson, S. Jha, C. Gupta, **D. Sarkar** and A. Singharoy, All You Want to Know About Large System Simulations, *Methods in Molecular Biology* -submitted, 2019 (role: corresponding author)

INVITED ABSTRACTS, TALK, PRESENTATION AND POSTERS

(* - equal contribution)

1. **D. Sarkar**, J. V. Vermaas, Tracking Photosynthetic Reactant and Product Diffusion Across Cyanobacterial Carboxysomes on Exascale Computing Platforms, Biophysics at the Dawn of Exascale Computers - Hamburg, Germany, Biophysical Society Thematic Meeting, 2022 - invited talk presented by J. V. Vermaas
2. **D. Sarkar**, J. L. Egelston, J. V. Vermaas Correlating the transport cycle of small multidrug resistance transporters, Annual Biophysical Society Meeting, 2022, *Biophysical Journal*, DOI: 10.1016/j.bpj.2021.11.800
3. F. T. Doole, C. K. Chan, E. Streitwieser, **D. Sarkar**, A. V. Struts, A. Singharoy, M.F. Brown, Rivalry of cholesterol and antimicrobial peptides as seen by molecular simulations and NMR spectroscopy, Annual Biophysical Society Meeting, 2022, *Biophysical Journal*, DOI: 10.1016/j.bpj.2021.11.1922
4. I. Santiago, **D. Sarkar**, J. V. Vermaas, Quantifying solvent impacts on lignin-cellulose interactions in diverse solvents, American Chemical Society, Fall 2021 meeting (virtual presentation).
5. **D. Sarkar**, M. Shekhar, A. Singharoy, 2021 EM Challenge Committee Meeting, Stanford University (invited talk, presented virtually).
6. G Terashi, C Christoffer, **D Sarkar**, D Kihara, Modeling SARS-CoV2 proteins in the CASP-commons experiment, CASP14-COVID 19 paper (invited abstract, manuscript in preparation), 2021.
7. C Christoffer, G Terashi, J Verburgt, **D Sarkar**, T Aderinwale, X Wang, D Kihara, Kihara human team and LZerD server in CAPRI 50 / CASP 14, (invited abstract, manuscript in preparation), *CAPRI50/CASP14 extended abstract*, 2021.
8. C Christoffer, G Terashi, J Verburgt, **D Sarkar**, T Aderinwale, X Wang, D Kihara, Kihara human team and LZerD server in CAPRI 50 / CASP 14, *CAPRI50/CASP14 extended abstract*, 2021.
9. **D. Sarkar**, J. Verburgt, C. Christoffer, Y. Kagaya, G. Terashi, K. Lundquist, X. Zhu, L. Gorenstein, D. Kihara, Integrative modeling for protein structure refinement using Molecular Dynamics with flat- bottom harmonic restraints, enhanced sampling and ROSETTA iterative hybridize, Critical Assessment of Structure Prediction (CASP 14), 2020 - virtual

conference. (Team leader invited to chair protein structure refinement session and to give oral presentation for protein cryoEM and NMR data guided modeling session).

10. G. Terashi, C. Christoffer, J. Verbugt, S. R. M. V. Subramanya, A. Jain, Y. Kagaya, **D. Sarkar**, T. Aderinwale, X. Wang, D. Kihara, Distance Prediction, Structure Prediction, Refinement, Quality Assessment, and Protein Docking in KiharaLab, Critical Assessment of Structure Prediction (CASP 14), 2020 - virtual conference.
11. F. Doole, C. K. Chan, E. Streitwieser, **D. Sarkar**, M. Kim, A. Singharoy, M. F. Brown, Antimicrobial peptide-Membrane interactions: Insights from Molecular Simulations, Annual Biophysical Society Meeting, 2021 - virtual Poster Presentation.
12. F. Doole, C. K. Chan, **D. Sarkar**, M. Kim, A. Singharoy, M. F. Brown, Antimicrobial Peptide Functionalized Biomaterials Investigated by Molecular Dynamics Simulations, Annual Biophysical Society Meeting 2020, San Diego, CA, USA - Poster Presentation.
13. **D. Sarkar**, R.D. Skeel and A. Singharoy, String like simulations outside the friction dominated regime, 4th NAMD Developers Meeting, Beckman Institute, University of Illinois Urbana-Champaign, Champaign, IL.
14. J.W. Vant, **D. Sarkar**, R.D. Skeel and A. Singharoy MDFF Error Analysis, 4th NAMD Developers Meeting, Beckman Institute, University of Illinois Urbana-Champaign, Champaign, IL, USA.
15. **D. Sarkar**, P. Kang, Z. Qin, Examining Arrhenius Kinetics over a Large Temperature Range, Summer Biomechanics, Bioengineering, and Biotransport (SB3C) Conference, June 2019, Seven Springs, Pennsylvania, USA - Invited talk for John Pearce 70th Birthday.
16. P. Kang, **D. Sarkar**, Z. Qin, Laser Fragmentation of Plasmonic Gold Nanoparticles: Coulomb Explosion versus Photothermal Evaporation, Summer Biomechanics, Bioengineering, and Biotransport (SB3C) Conference, June 2019, Seven Springs, Pennsylvania, USA - Poster Presentation.
17. **D. Sarkar**, J. W. Vant, M. Shekhar, J. S. Richardson, R. Skeel, A. Singharoy, MDFF Error Analysis: A Tool for Determining Stereochemical and Thermodynamic Correct Structures, Biophysical Journal, 116, 3, supp. 1, 140A-141A (694-Pos) – Annual Biophysical Society Meeting 2019, Baltimore, MD.
18. **D. Sarkar**, P. Kang, S. O. Nielsen, Z. Qin, Reaction-Diffusion Kinetics During Selective Photo-Inactivation of Proteins by Molecular Hyperthermia, NEMB2018-6203, ASME 2018 NanoEngineering for Medicine and Biology Conference (NEMB), August 21 -24, 2018, Los Angeles, CA.
19. **D. Sarkar**, P. Kang*, Z. Qin, Molecular Hyperthermia to Manipulate Individual Proteins: Feasibility and Non-Arrhenius Kinetics, 8th World Congress of Biomechanics, 8-12 July 2018, Dublin, Ireland - Oral presentation.
20. P. Kang, **D. Sarkar**, T. Price, Z. Qin, Molecular Hyperthermia: the final frontier of biothermal science, Photo thermal effects in plasmonics (PEP18), Summer School, Special focus on biology, June 24-29, 2018, Porquerolles island, France.
21. **D. Sarkar**, P. Kang*, S.O. Nielsen, Z. Qin, Non-Arrhenius Reaction-Diffusion Kinetics for Protein Unfolding, Inactivation and Inhibition Over a Large Temperature Range, The

Bluebonnet Symposium on Thermal-Fluid Sciences, 27 April 2018, The University of Texas at Dallas, Richardson, TX, USA – Invited talk.

22. R. Raj, **D. Sarkar**, A. Jain, Thermal modelling of memory access operations in micro-processors, Proc. ASME 2016 International Mechanical Engineering Congress and Exposition, IMECE2016-67697, November 11-17, Phoenix, AZ, USA 2016.
23. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Thermal transport in perfused biological tissue due to gold/magnetic nanoparticle heating, ASME NEMB 2016 Nano-Engineering for Medicine and Biology Conference, NEMB2016-6118, February 21-24, Houston, TX, USA 2016.
24. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Theoretical analysis of transient bio-heat transfer in multi-layer tissue, Proc. ASME 2015 International Mechanical Engineering Congress and Exposition, IMECE2015-53392, November 13-19, Houston, TX, USA 2015.
25. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Analytical temperature distribution in a multilayer tissue structure in the presence of a tumor, Proc. ASME 2013 International Mechanical Engineering Congress and Exposition, IMECE2013-63275, November 15- 21, San Diego, CA, USA 2013.

AWARDS

Doctoral Dissertation Fellowship, College of Engineering, The University of Texas at Arlington, 2016 (awarded annually by the College of Engineering to selected Doctoral bound students)

Research Internships in Science and Engineering fellowship, Indo-US Science and Technology Forum, 2015

Enhanced Graduate Teaching Assistant, Mechanical and Aerospace Engineering Department, The University of Texas at Arlington (awarded annually by the College of Engineering to selected Doctoral bound students)

ACADEMIC MENTORSHIP

Jessica Egelston, Department of Biochemistry and Molecular Biology, Michigan State University
- XSEDE-EMPOWER Fellowship, Spring 2022

Ian Santiago, Senior Undergraduate, Louisiana State University, Baton Rouge, LA
- XSEDE-EMPOWER Fellowship, Fall 2021
- Michigan State University Summer Research Opportunities Program (MSU-SROP)

Ellen Strietweiser, Arizona State University (current position: PhD student in University of Washington, Seattle)

Divya Chalise, University of Texas at Arlington (current position: PhD student in University of California, Berkeley)

WORKSHOPS

NAMD Developers meeting, UIUC, IL - September 2021

NAMD Developers meeting, UIUC, IL - August 2019

Free Energy and Enhanced Sampling with NAMD, UIUC, IL – September 2017

Molecular Dynamics with LAMMPS, Temple University, PA – August 2016