# Siva Dasetty, PhD

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## Education

- **Postdoctoral Associate, Molecular Engineering** — **The University of Chicago, Chicago, IL**
  *Advisor: Prof. Andrew L. Ferguson* — *Mar. 2020–Present*
- **PhD, Chemical Engineering** — **Clemson University, Clemson, SC**
  *Advisor: Prof. Sapna Sarupria* — *Aug. 2019*
- **MS, Chemical Engineering** — **Clemson University, Clemson, SC**
  *Advisor: Prof. Sapna Sarupria* — *Aug. 2015*
- **BTech, Chemical Engineering** — **NITK Surathkal, India**
  *May 2012*

## Research Experience

**Postdoctoral Associate** — **Ferguson Lab, The University of Chicago, Chicago, IL**

Pritzker School of Molecular Engineering (PME) — Mar. 2020–Present

- Inverse design of materials using molecular simulations, enhanced sampling methods and machine learning.
  1. Worked with experimentalists to engineer nanostructured materials composed of dielectric particles.
  2. Applied active learning to efficiently map 2-particle phase diagrams along experimental design parameters for guiding the design of self-assembling superlattices composed of dielectric particles.
- Leading efforts to incorporate enhanced sampling methods and collective variables to the enhanced sampling software SSAGES and PySAGES.
- Contributed to the development of a neural network collective variable and its implementation in the enhanced sampling software PLUMED for probing solvent effects in various molecular systems.
- Applying a novel machine learning solution to efficiently remove organic water contaminants.
- Assisting mentoring of current graduate students in Ferguson lab – Max Topel (PhD candidate in Physics, U.Chicago) and Nicholas Herringer (PhD candidate in PME, U.Chicago).

**Graduate Research Assistant** — **Sarupria Group, Clemson University, Clemson, SC**

Department of Chemical Engineering — May 2014–Aug. 2019

- Advanced engineering of proteins and protein–surface complexes using statistical mechanics theory and molecular simulations.
  1. Partnered with experimentalists to engineer low temperature activity in a model thermophilic lipase.
     - Analyzed the correlation between changes in dynamics and activity of a thermophilic lipase with mutation.
     - Identified critical residues that altered the structure of enzyme with mutation using network theory.
  2. Elucidated the role of context of a residue in peptide–graphene interactions.
     - Assessed the differences in the adsorption of amino acids on graphene with force fields.
     - Developed a protocol to identify predominant peptide configurations in adsorbed state using principal component analysis and density based clustering algorithm.
  3. Developed a Python program to generate all-atom cross-linked polyamide structure.
- Mentored students and led several group meetings in Sarupria group.
  - Led the training in Sarupria group on the best practices in molecular simulations. This involved in depth

discussions and review of relevant literature.

- Mentored John K. Barrows during his undergraduate research in molecular simulations at Sarupria group. The collaborative effort resulted in one publication. After graduation, John started his PhD at the Medical University of South Carolina.
- Mentored Salman B. Kashif in developing multiscale methods for designing foulant-resistance membranes. Salman is currently a PhD candidate in Chemical Engineering at Clemson University.
- Mentored Diego Losada Rubio (undergraduate student in Physics, Wofford college) during summer of 2019 on the basics and best practices in molecular simulations.

**Undergraduate Research Assistant** **Ayappa Lab, Indian Institute of Science, India**

Department of Chemical Engineering Aug. 2011–Dec. 2011

- Investigated heat effects during charging and discharging of adsorbed natural gas (ANG) from activated carbon bed.
  1. Obtained numerical solutions of a 2D axisymmetric model describing the heat effects of ANG system.
  2. Reduced computational cost of the 2D model by developing an effective 1D lumped parameter model.

## Teaching Experience

**Graduate Teaching Assistant** **Clemson University, Clemson, SC**

Department of Chemical Engineering Aug. 2013–May 2014

- CHE 4500 – Chemical Reaction Engineering (Fall 2013)

  Assisted Prof. Mark A. Blenner in teaching undergraduate Chemical Reaction Engineering course (CRE) to forty three senior-year students at Clemson University. This is one of the core courses in chemical engineering that introduces students to the design and analysis of batch as well as continuous chemical reactors for either homogeneous or heterogeneous reactions.

- CHE 2300 – Fluids & Heat Transfer (Spring 2014)

  Assisted my PhD advisor Prof. Sapna Sarupria in teaching Fluids & Heat Transfer course to fifty one sophomore students at Clemson University. This is another important chemical engineering course that introduces students to fundamental principles of fluid dynamics and heat transfer such as continuity equation, momentum balance and energy balance.

## Industrial Experience

**Associate Software Engineer** **Exeter (part of Exeter Group, Boston), India**

mscripts team May 2012–Jun. 2013

- Software developer in mscripts team that focused on facilitating patients–healthcare provider connection using a mobile application.
  1. Developed a tool using JavaScript, HTML and SQL to track the number of active customers on a webpage with user specified conditions.
  2. Worked with associates to resolve client-defined issues.

## Publications

### Published


[1] **Dasetty, S.**, Coropceanu, I., Portner, J., Li, J., de Pablo, J. J., Talapin, D., and Ferguson, A. L., "Active learning of polarizable nanoparticle phase diagrams for the guided design of triggerable self-assembling superlattices," *Molecular Systems Design & Engineering*, 2022.

[2] **Dasetty, S.** and Sarupria, S., "Advancing rational control of peptide–surface complexes," *J. Phys. Chem. B*, vol. 125, no. 10, pages 2644–2657, 2021,
— Featured in the supplementary cover of *J. Phys. Chem. B*, Vol. 125, Issue 10. (Mar. 18, 2021).

[3] Wang, W., **Dasetty, S.**, Sarupria, S., and Blenner, M., "Rational engineering of low temperature activity in thermoalkalophilic geobacillus thermocatenulatus lipase," *Biochem. Eng. J.*, page 108 093, 2021.

[4] **Dasetty, S.**, Barrows, J. K., and Sarupria, S., "Adsorption of amino acids on graphene: Assessment of current force fields," *Soft Matter*, vol. 15, no. 11, pages 2359–2372, 2019.

[5] **Dasetty, S.**, Meza-Morales, P. J., Getman, R. B., and Sarupria, S., "Simulations of interfacial processes: Recent advances in force field development," *Curr. Opin. Chem. Eng.*, vol. 23, pages 138–145, 2019.

[6] **Dasetty, S.**, Blenner, M. A., and Sarupria, S., "Engineering lipases: Walking the fine line between activity and stability," *Mater. Res. Express*, vol. 4, no. 11, page 114 008, 2017.

[7] Sengupta, B., Gregory, W. E., Zhu, J., **Dasetty, S.**, Karakaya, M., Brown, J. M., Rao, A. M., Barrows, J. K., Sarupria, S., and Podila, R., "Influence of carbon nanomaterial defects on the formation of protein corona," *RSC Adv.*, vol. 5, no. 100, pages 82 395–82 402, 2015.

[8] Sahoo, P., Prajwal, B., **Dasetty, S.**, John, M., Newalkar, B., Choudary, N., and Ayappa, K., "Influence of exhaust gas heating and ld ratios on the discharge efficiencies for an activated carbon natural gas storage system," *Appl. Energ.*, vol. 119, pages 190–203, 2014,
— Work performed as an undergraduate student. Developed the lumped parameter model (described in Section 4).

## Presentations

### Oral Presentations

- **Dasetty, S.**, Coropceanu, I., Portner, J., Li, J., de Pablo, J. J., Talapin, D. V., and Ferguson, A. L., *Coarse-grained modeling of polarizable nanoparticle assembly*, AIChE Annual Meeting, Boston, MA, 2021.
- **Dasetty, S.**, Topel, M., Wang, Y., Rowan, S. J., Lee, S. S., Darling, S. B., Benmore, C. J., Willet, R., Jonas, E., Chen, J., and Ferguson, A. L., *Inverse design of molecular probes to bind with water contaminants*, AIChE Annual Meeting, Boston, MA, 2021.
- **Dasetty, S.**, Dhanasekaran, J., Li, J., de Pablo, J. J., and Ferguson, A. L., *Enhanced sampling and inverse design of self-assembling patchy and polarizable colloids*, AIChE Annual Meeting, Virtual Platform, 2020.
- **Dasetty, S.**, Hilbert, M., A, B. M., and Sarupria, S., *Predictive structure-function relationship for enzymes immobilized on complex surfaces*, DTRA Life Sciences Technical Review, Woodbridge, VA, 2019.
- **Dasetty, S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Towards computer aided engineering of proteins and protein–surface complexes in aqueous media*, Chemical Engineering Graduate Symposium, Clemson, SC, 2018.
- **Dasetty, S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Controlling working temperatures of enzymes using rational approaches*, Graduate Research and Discovery Symposium, Clemson, SC, 2018.
- **Dasetty, S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Engineering robust activity in extremophilic enzymes*, AIChE Annual Meeting, Minneapolis, MN, 2017.
- **Dasetty, S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Engineering robust activity in extremophilic enzymes*, Chemical Engineering Graduate Symposium, Clemson, SC, 2017.
- **Dasetty, S.**, Barrows, J. K., and Sarupria, S., *Binding affinities of amino acids on graphene: Assessment of force fields*, AIChE Annual Meeting, San Francisco, CA, 2016.
- **Dasetty, S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Understanding the structural differences between psychrophilic and thermophilic enzymes: A molecular dynamics study*, AIChE Annual Meeting, San Francisco, CA, 2016.
- **Dasetty, S.** and Sarupria, S., *Role of protein sequence in driving molecular interactions between proteins and carbon nanomaterials: A molecular dynamics study*, AIChE Annual Meeting, Salt Lake City, UT, 2015.

### Poster Presentations

- **Dasetty, S.**, Coropceanu, I., Portner, J., Li, J., de Pablo, J. J., Talapin, D. V., and Ferguson, A. L., *Machine learning assisted design of switchable self-assembling materials*, PME $10^{th}$ Anniversary, University of Chicago, 2021,
  — Won best poster award in the category "Presentation Best Highlighting Collaboration Across Thematic Areas".
- Herringer, N., **Dasetty, S.**, and Ferguson, A. L., *Discovery and direct enhanced sampling of solvent-inclusive atomistic cvs using autoencoder embeddings*, RARE, 2021.
- **Dasetty, S.** and Sarupria, S., *Advancing rational design of peptide self-assembly at surfaces*, AIChE Annual Meeting, Virtual Platform, 2020.
- **Dasetty S.**, Hilbert, M., Blenner, M. A., and Sarupria, S., *Developing efficient enzyme immobilization strategies by studying model enzyme-linker-surface complexes*, DTRA Life Sciences Technical Review, Springfield, VA, 2018.
- **Dasetty S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Engineering low temperature activity in thermophilic enzymes*, Protein Folding Dynamics Gordon Research Conference, Galveston, TX, 2018.
- **Dasetty S.**, Hilbert, M., Blenner, M. A., and Sarupria, S., *Impact of linker attachment site on structure and dynamics of enzymes*, DTRA Life Science Technical Review, Lorton, VA, 2017.
- **Dasetty S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Engineering low temperature activity in thermophilic enzymes*, AIChE Annual Meeting, Minneapolis, MN, 2017.
- **Dasetty S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Engineering robust activity in extremophilic enzymes*, Clemson Biological Sciences Annual Student Symposium, Biological Sciences, Clemson University, Clemson, SC, 2017.
- **Dasetty S.**, Wang, W., Blenner, M. A., and Sarupria, S., *Engineering robust activity in extremophilic enzymes*, The Future of Integrative Structural Biology, Physics, Clemson University, Clemson, SC, 2017.

## Memberships

- American Institute of Chemical Engineers — Oct. 2015–Present
- Materials Research Society — Oct. 2021–Present
- Chemical Engineering Graduate Student Organization, Clemson University — Aug. 2013–Aug. 2019

## Awards

- Awarded $250 for the research poster best highlighting collaboration across research areas during PME Anniversary, University of Chicago in Sept. 2021.
- Awarded $750 for professional enrichment by Graduate Student Government, Clemson University in Sept. 2016.

## Extracurricular Activities

**Volunteer** — **Regional National Science Bowl (NSB) Competetion, IL**

Jan. 2022

Middle School NSB is a nationwide competetion that tests students' knowledge in all areas of science and mathematics supported by the United States Department of Energy. I am one of the volunteer recognizer and scorekeeper to run the competition smoothly by acknowledging students who raise their hand during the event and tracking official scores.

**Volunteer** — **Peer Lab Walkthrough Competition, University of Chicago, IL**

May 2021

Volunteered as a judge for the peer lab walkthrough competition, which is a collaborative educational opportunity for labs to trade safety knowledge, creative fixes, and learned lessons. Provided assessment of the lab organization and safety protocols.

**Volunteer** **First Lego League, Tri-county Technical College, SC**

Jan. 2016

First Lego League is a competition designed to develop focus and research experience in elementary and middle school students. Provided assistance in various areas such as distributing pins, medals, and trophies as determined by the manager of event day volunteer.

**Volunteer** **Girls Scouts Event, Clemson University, SC**

Feb. 2016

Assisted in setting up polymer-based experiments to teach and demonstrate basics of polymers to middle and early high school girls.

## Technical Skills

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| Programming Languages: | Python (Numpy, Scikit-Learn, SciPy, Jupyter lab, Pandas, SQLite, Matplotlib, PyTorch, GPyTorch, BoTorch, RDKit), C++, Scripting (bash, Apple, TCL), LaTeX. |
| Other Languages and Software: | GROMACS, LAMMPS, MATLAB, R, COMSOL Multiphysics, VMD, Ovito, Chimera, Cytoscape, Microsoft Applications (Excel, Word, PowerPoint), Keynote, Blender, Adobe Photoshop. |
| Operating Systems & Platforms: | Mac OS, Linux, Windows, High-performance computing (PBS and SLURM). |

## Coursework in Graduate School

Probability, Data Analysis, Advanced Numerical Methods, Multiscale Modeling, Computational Chemistry, Advanced Transport Phenomena, Biomolecular Engineering, Chemical Engineering Kinetics, Chemical Engineering Thermodynamics, Computational Chemistry, Mathematical Programming, Polymer Thermodynamics, Polymers, Scientific Computing, Statistical Thermodynamics.