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Siddarth K. Achar

Education and Training

2024 - present **University of Chicago**, Chicago, IL
Postdoctoral Research Associate
Advisors: Andrew Ferguson and Junhong Chen

2020 - 2024 **University of Pittsburgh**, Pittsburgh, PA
Ph.D. in Computational Modeling and Simulation
Advisor: J. Karl Johnson

2018 - 2019 **Carnegie Mellon University**, Pittsburgh, PA
M.S. in Chemical Engineering
Advisor: John Kitchin

2014 - 2018 **R.V. College of Engineering**, Bangalore, India
B.E. in Chemical Engineering
Research Project Mentor: R. J. Basavaraja

Awards and Honors

2024 **Travel Award**, Foundations of Molecular Modeling and Simulation (FOMMS) Travel Award, FOMMS

2024 **APS Group Data Science IMPACT Award**, American Physical Society

2024 **Dr. Jim Pommershiem Graduate Student Fellowship Award**, University of Pittsburgh - Chemical Engineering

2023 **AIChE Computational Molecular Science & Engineering Forum (CoMSEF) Outstanding Graduate Student Award**, American Institute of Chemical Engineers

2023 **Dr. James Coull Memorial Best Student Award Fellowship**, University of Pittsburgh – Chemical Engineering

2023 **Research Assistant of the Year Award**, University of Pittsburgh – Chemical Engineering

2023 **Advances in Research Computing Poster Award**, University of Pittsburgh – Center for Research Computing

2022 **Graduate Student Fellowship**, Pittsburgh Quantum Institute

2022 **Best Overall Student Poster Award**, Pittsburgh Quantum Institute

2022 **Best Poster in Swanson School of Engineering Award**, Pittsburgh Quantum Institute

2022 **Uni-Pro Initiative Award**, Pittsburgh Quantum Institute

2023 **APS GERA Workshop Travel Award**, APS March

2019 **Hackathon Winner 3rd Place**, SDLC Partners 2019 Hackathon, Pittsburgh

2018 **Best Innovative Project Award**, R.V. College of Engineering, EDC Development

2018 **Project Sponsorship**, Karnataka State Council for Science and Technology

2017 **Summer Research Fellowship**, Saha Institute of Nuclear Physics

Publications

1 He, Y., De Souza, M., Luo, T., **Achar, S. K.**, Johnson, K. J., Rosi, N. L. (2024). Leveraging Ligand Steric Demand to Control Ligand Exchange and Domain Composition in Stratified Metal-Organic Frameworks. *Angewandte Chemie International Edition*, e202409150. [Link]

2 **Achar, S. K.**, Bernasconi, L., Alvarez, J. J., & Johnson, J. K. (2023). Deep-learning potentials for proton transport in double-sided graphanol. *Journal of Materials Research*, 1-11. [Link]

3 **Achar, S. K.**, Bernasconi, L., & Johnson, J. K. (2023). Machine Learning Electron Density Prediction Using Weighted Smooth Overlap of Atomic Positions. *Nanomaterials*, 13(12), 1853. [Link]

4 **Achar, S. K.**, Bernasconi, L., DeMaio, R. I., Howard, K. R.,& Johnson, J. K. (2023). In Silico Demonstration of Fast Anhydrous Proton Conduction on Graphanol. *ACS Applied Materials & Interfaces*, 15, 21, 25873–25883. [Link]

5 **Achar, S. K.**, Stewart, D.& Schneider, J. (2022). Using Machine Learning Potentials to Explore Interdiffusion at Metal-Chalcogenide Interfaces. *ACS Applied Materials and Interfaces*. [Link]

6 **Achar, S. K.**, Wardzala, J. J., Bernasconi, L., Zhang, L.,& Johnson, J. K. (2022). Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66. *Journal of Chemical Theory and Computation*, 18, 3593-3606. [Link]

7 Yang, Y., **Achar, S. K.**,& Kitchin, J. R. (2022). Evaluation of the degree of rate control via automatic differentiation. *AIChE Journal*, 68(6), e17653. [Link]

8 **Achar, S. K.**, Zhang, L.,& Johnson, J. K. (2021). Efficiently trained deep learning potential for graphane. *The Journal of Physical Chemistry C*, 125(27), 14874-14882. [Link]

9 Madathil, A. P., **Achar, S. K.**, Moses, V., Meda, U. S., Chetan, N., Vidya, C., ...& Sarode, M. (2020). Use of Keratin Present in Chicken feather as a Hydrogen Storage Material: A Review. *International Journal of Engineering Materials and Manufacture*, 5(4), 148-155. [Link]

10 **Achar, S. K.**, Madathil, A. P., Naveen C., Gosh, B.,& Phani, A R (2018). Thickness Dependent Optical Properties of Sol-gel based MgF2 – TiO2 Thin Films. *Journal Article Mechanics, Materials Science & Engineering*, 179(52), 2412-5954. [Link]

Conference Proceedings

11 Gupta, S., Bonageri, S., **Achar, S. K.**,& Menon, A. (2018, May). Synthesis of porous graphene powder through improved Hummers' method. In *AIP Conference Proceedings* (Vol. 1966, No. 1, p. 020014). AIP Publishing LLC. [Link]

In Preparation

12 **Achar, S. K.**, Shukla, P. B., Mhatre, C. V., Vinger, C. Y., Johnson, K. J. (2024). Reactive Active Learning for Machine Learning Potentials using Growing Strings, *in preparation*

13 **Achar, S. K.**, Bernasconi, L., Johnson, K. J. (2024). Identifying Proton-Coupled Electron Transfer using Machine Learning Electron Densities, *in preparation*

14 Ananthabhotla, L.Y., **Achar, S. K.**, Johnson, K. J. (2024). Anhydrous Proton Transfer in Graphamine: Deep Learning Potential Investigation, *in preparation*

Professional Experience

May 2021 – Aug 2021 **RAMP Computational Material Science Intern**, *Western Digital*
Formulated a new machine learning (ML) inter-atomic force fields-based workflow using moment tensors and density functional theory (DFT) to discover stable non-volatile memory cells.

May 2022 – Aug 2022 **Computational NVM Development Intern**, *Western Digital*
Designed novel phase-change memory alloy interfaces using ML force fields that showed enhanced stability for over 10 ns.

Academic Research Experience

Aug 2024 – present **Postdoctoral Research Associate**, *University of Chicago*

- Developing a Bayesian Optimization workflow combined with generative artificial intelligence (AI) models and molecular mechanics for high-throughput screening of molecular probes for the detection of forever chemicals.

Jan 2020 – Jul 2024 **Graduate Student Researcher**, *University of Pittsburgh*

- Designed ML potentials with deep learning (DL) to model a graphane-based material for proton conduction; 6x more effective than conventional fuel cell membranes.
- Discovered the "Grotthuss Chain" phenomena using DL and lattice Monte Carlo simulations and proposed new direction for fuel cell membrane development based on this mechanism.
- Reactive Active Learning (RAL): Developed a workflow that uses the growing string method, generative AI, and DFT to build accurate reaction-aware machine learning force fields.
- Demonstrated RAL to have higher data-efficiency and accuracy than traditional active learning schemes. Tested RAL on gas-phase and catalytic reactions.
- Designed DeepCDP, a python package to generate DL models for electron density predictions using weighted-SOAP descriptors and achieved $> 99\%$ prediction accuracy with linear scaling.
- Identified proton coupled electron transfer reactions using dipole fluctuation predictions from DeepCDP.
- Formulated a hybrid potential approach to MD by combining DL and classical potentials to compute guest atom diffusion in metal-organic frameworks (MOFs) implemented on LAMMPS.

Jan 2019 – Dec 2019 **Graduate Student Researcher**, *Carnegie Mellon University*

- Developed automatic differentiation-based methods to calculate DRC for multi-step catalytic reactions, showing superiority over finite differences; proposed hybrid sensitivity analysis for kinetic parameter assessment.
- Designed a novel Meta-Gradient Adversarial Attack (MGAA) attack methodology for deep learning-based speech recognition, previously used only in image recognition to increase model robustness on adversarial attacks.

Jan 2018 – May 2018 **Undergraduate Research Project**, *R.V. College of Engineering*

- Development of Graphene Based Post-Combustion CO_2 Capture System: Reduced graphene production cost by 30% via Hummer's process; tested adsorption capacity with CO_2 and N_2 in patent-published study using augmented fluid jacket column.

Teaching, Mentoring & Service

Aug 2022 – Dec 2022 **Teaching Assistant**, *University of Pittsburgh*, CHE-2201: Fundamentals of Reaction Processes

Gave two lectures on modeling chemical reactors using numerical solvers and one lecture on computational chemistry.

Nov 2023 **Guest Lecture**, *University of Pittsburgh*, CHE 3460: Advanced Scientific Visualization

Sept 2024 – present **Undergraduate Student Mentoring**, *University of Chicago*

Mentoring a UChicago bio + data science undergraduate student.

Aug 2020 – present **Undergraduate Student Mentoring**, *University of Pittsburgh*

Mentored 4 students, leading to research publications (published + under review).

May 2023 – present **President**, *ChE Graduate Student Association, University of Pittsburgh*

Organized two ChE department research symposiums.

Jan 2020 – present **Academic peer-review**

Peer-reviewed the following research journals: ACS: J. Phys. Chem., J. Chem. Theory Comput, AMI, Appl. Mater. Interfaces, Matt. Lett., Omega; Wiley: ChemPlusChem, Medical Physics Journal; Spinger: EPJP, Nature: Scientific Reports.

Jan 2019 – Dec 2019 **Social Chair**, *ChE Graduate Student Association, Carnegie Mellon University*

Organized weekly social events for ChE gradudate students, postdocs, and faculty.

Aug 2017 – May 2018 **President and Treasurer**, *RVQuizCorp, R.V. College of Engineering*

Organized several national quiz tournaments. Organized Sweden India Nobel Memorial Quiz, 2017.

Presentations

31 S. Achar, L. Bernasconi, J. K. Johnson. Reaction-aware machine learning potentials using growing string method-based active learning, Foundations of Molecular Modeling and Simulation (FOMMS), (2024), Snow Bird, UT.

30 S. Achar, L. Bernasconi, J. K. Johnson. Machine Learning Electron Density Prediction using Weighted Smooth Overlap of Atomic Positions, American Chemical Society (ACS), (2024), New Orleans, LA.

29 S. Achar, P. Shukla, C. Vinger, C. Mhatre, L. Bernasconi, J. K. Johnson. Reaction-aware machine learning potentials using growing string method-based active learning, American Chemical Society (ACS), (2024), New Orleans, LA.

28 S. Achar, L. Bernasconi, J. K. Johnson. Catalyzing Anhydrous Proton Conduction: A Computational Workflow for Fuel Cell Materials Design Electrochemical Energy Conversion, American Physical Society (APS March), (2024), Minneapolis, MN.

27 S. Achar, J. K. Johnson. From Electron Density to Fuel Cells with Molecular Machine Learning. Yue Research Lab, Cornell University (2023), (Invited Talk), Ithaca, NY.

26 S. Achar, J. Wardzala, L. Bernasconi, L. Zhang, J. K. Johnson. A Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66, American Institute of Chemical Engineers (AIChE) Annual, (2023), Orlando, FL.

25 S. Achar, L. Bernasconi, J. K. Johnson. Machine Learning with Weighted-Soap to Efficiently Predict Electron Densities, American Institute of Chemical Engineers (AIChE) Annual, (2023), Orlando, FL.

24 S. Achar, L. Bernasconi, J. K. Johnson. Using Deep Learning Potentials and Graph Lattice Models to Engineer Optimal Proton Conducing Membranes for Fuel Cells, American Institute of Chemical Engineers (AIChE), (2023), Orlando, FL.

23 S. Achar, L. Bernasconi, J. K. Johnson. Using Deep Learning Potentials and Graph Lattice Models to Engineer Optimal Proton Conducing Membranes for Fuel Cells, American Chemical Society, (2023), San Francisco, CA.

22 S. Achar, L. Bernasconi, J. K. Johnson. Using Deep Learning Potentials and Graph Lattice Models to Engineer Optimal Proton Conducing Membranes for Fuel Cells, Pitt CRC ARC, (2023), Pittsburgh, PA.

21 S. Achar, L. Bernasconi, J. K. Johnson. Advancements in Graphene-based materials for Anhydrous Proton Conduction: An atomistic study, Pitt ChE Research, (2023), Pittsburgh, PA.

20 S. Achar, L. Bernasconi, J. K. Johnson. DeepCDP: Deep Learning Charge Density Prediction, American Institute of Chemical Engineers (AIChE) Annual, (2022), Phoenix, AZ.

19 S. Achar, J. Wardzala, L. Bernasconi, L. Zhang, J. K. Johnson. A Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66, American Institute of Chemical Engineers (AIChE) Annual, (2022), Phoenix, AZ.

18 S. Achar, L. Bernasconi, L. Zhang, J. K. Johnson. Studying Anhydrous Proton Conduction on Graphene-Based Materials Using Deep Learning Methods, American Institute of Chemical Engineers (AIChE) Annual, (2022), Phoenix, AZ.

17 S. Achar, D. Stewart, J. Schneider. Using Machine Learning Empirical Potentials to Investigate Interdiffusion at Metal-Chalcogenide Alloy Interfaces, Materials Science & Technology (MS&T) Fall, (2022), Pittsburgh, PA.

16 S. Achar, L. Bernasconi, L. Zhang, J. K. Johnson. Design of Graphene-Based Anhydrous Proton Conducting Materials Using Deep Learning Methods, Pittsburgh Quantum Institute (PQI) 2022, Pittsburgh, PA.

15 S. Achar, L. Bernasconi, L. Zhang, J. K. Johnson. Design of Graphene-Based Anhydrous Proton Conducting Materials Using Deep Learning Methods, University of Pittsburgh Research Day, (2022), Pittsburgh, PA.

14 S. Achar. Machine Learning and Quantum Mechanics to Study Particle Transport, Center for Hydrogen and Green Technology (CH2GT), R.V. College of Engineering, (2022) (Invited Talk), Bangalore, India.

13 S. Achar, L. Zhang, L. Bernasconi, J. K. Johnson. Studying Anhydrous Proton Transport on Graphene-based Materials using Deep Learning Methods, Materials Research Society (MRS) Spring, (2022), (Virtual).

12 S. Achar, L. Zhang, L. Bernasconi, J. K. Johnson. Studying Anhydrous Proton Transport on Graphene-based Materials using Deep Learning Methods, American Chemical Society (ACS) Spring, (2022), San Diego, CA.

11 S. Achar, D. Stewart, J. Schneider. Using machine learning empirical potentials to investigate interdiffusion at metal-chalcogenide alloy interfaces, Materials Research Society (MRS) Fall, (2021), Boston, MA.

10 S. Achar, L. Zhang, L. Bernasconi, J. K. Johnson. Studying Anhydrous Proton Transport on Graphene-based Materials using Deep Learning Methods, Psi-k ML-IP workshop, (2021), (Virtual).

9 S. Achar, L. Zhang, L. Bernasconi, J. K. Johnson. Studying Anhydrous Proton Transport on Graphene-based Materials using Deep Learning Methods, American Institute of Chemical Engineers (AIChE) Annual, (2021), Boston, MA.

8 S.Achar, J. Wardzala, L. Zhang, L. Bernasconi, J. K. Johnson. A Neural Network and Lennard-Jones Hybrid Forcefield to Study Diffusion of Neon in UiO-66, Advancing Research Through Computing (ARC), (2021), Pittsburgh, PA.

7 J. K. Johnson, S. Achar. Studying Anhydrous Proton Transport on Graphene-based Materials using Deep Learning Methods, Ohio State University (Invited), (2021), Columbus, OH.

6 S. Achar, L. Zhang, J K. Johnson. Towards a deep learning potential for anhydrous proton transport, American Institute of Chemical Engineers (AIChE) Annual, (2020), San Francisco, CA.

5 S. Achar, L. Zhang, J K. Johnson. Towards a deep learning potential for anhydrous proton transport, Pittsburgh Quantum Institute, (2020), Pittsburgh, PA.

4 S. Achar, J. R. Kitchin. Calculation of Degree of Rate control for multistep reactions at steady and unsteady state, Pittsburgh-Cleveland Catalysis Society Conference, (2019), Pittsburgh, PA.

3 S. Achar, J. R. Kitchin. Calculation of Degree of Rate control for multistep reactions at steady and unsteady state, 41st Annual ChEGSA Symposium, Carnegie Mellon University, (2019), Pittsburgh, PA.

2 S. Achar, S. Gupta, S. Bonageri, B.R.J. Synthesis of porous graphene powder through improved Hummers' method, American Institute of Physics (AIP) Conference, (2018), Coimbatore, Tamil Nadu, India.

1 S. Achar, A. PM, C.S. Naveen, B. Ghosh, A.R. Phani. Thickness dependent optical properties of TiO2-MgF2 nanocomposite thin films by using Envelope technique, International Conference on Advances in Materials Science and Technology, (2017), VIT Vellore, Tamil Nadu, India.

Patents

1 1. R J, Basavaraja, Gupta, Siddhant, Achar, Siddarth, Bonageri, Shrilakshmi, Menon, Atul. Fluid Jacketed Temperature Swing Adsorption System for Carbon Dioxide Capture Using Graphene. India. 202041024611, September 2022

Skills

Programming Languages: Python (PyTorch, Tensorflow), C++, MATLAB, Unix shell script (Git)

Computational Chemistry Tools: CP2K, VASP, LAMMPS, GROMACS, Gaussian, DeePMD, QuantumATK, RDKit, Blender, PySCF, PyMOL

Other Software: Aspen Plus, UniSim, COMSOL Multiphysics, GAMS

HPC Related: MPI, OpenMP, pthreads, OpenACC

Professional Membership

- American Institute of Chemical Engineers (CoMSEF), 2017 – Present
- American Chemical Society (COMP), 2020 – Present
- American Physical Society (DCOMP, GDS, GERA), 2024 – Present
- Materials Research Society, 2021 – Present