Siddarth K. **Achar**

Ph.D. Student in Computational Modeling and Simulation | University of Pittsburgh
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Education

University of Pittsburgh, Pittsburgh, PA **GPA: 3.85/4.00**
Ph.D. in Computational Modeling and Simulation (*Advised by Dr. J. Karl Johnson*) Jan 2020 – Jun 2024 (expected)

Carnegie Mellon University, Pittsburgh, PA **GPA: 3.80/4.00**
Master of Science in Chemical Engineering (*Advised by Dr. John Kitchin*) Aug 2018 – Dec 2019

R.V. College of Engineering (RVCE), Bangalore, India **GPA: 9.15/10.00**
Bachelor of Engineering in Chemical Engineering Aug 2014 - May 2018

Awards and Honors

APS Group Data Science IMPACT Award, *American Physical Society* 2024
AIChE Computational Molecular Science &Engineering Forum (CoMSEF) Outstanding Graduate Student Award, *American Institute of Chemical Engineers* 2023
Dr. Jim Pommershiem Graudate Student Fellowship Award, *University of Pittsburgh – Chemical Engineering* 2024
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* 2023
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* 2022
APS GERA workshop Travel Award, *APS March* 2023
Hackathon Winner 3rd place, *SDLC Partners 2019 Hackathon*, Pittsburgh. 2019
Best Innovative Project Award, *R.V. College of Engineering*, EDC Development. 2018
Project sponsorship, *Karnataka State Council for Science and Technology* 2018
Summer Research Fellowship, *Saha Institute of Nuclear Physics* 2017

Publications (with hyperlinks)

Published work

1. **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)
2. **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)
3. **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)
4. **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)
5. **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)
6. 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)
7. **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)

8. 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).
9. **Achar, S. K.,** Madathil, A. P., S., 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

10. 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

11. **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**.**
12. **Achar, S. K.,** Bernasconi, L., Johnson, K. J. (2024). Identifying Proton-Coupled Electron Transfer using Machine Learning Electron Densities.
13. Ananthabhotla, L.Y., **Achar, S. K.,** Johnson, K. J. (2024). Anhydrous Proton Transfer in Graphamine: Deep Learning Potential Investigation.

Professional Experience

Western Digital

- RAMP Computational Material Science Intern — May 2021-Aug 2021
- Computational NVM Development Intern — May 2022-Aug 2022

- Formulated a new machine learning (ML) inter-atomic forcefields-based workflow using moment tensors and density functional theory (DFT) to discover stable non-volatile memory cells.
- Designed novel phase-change memory alloy interfaces using ML forcefields that showed enhanced stability for over 10 ns.

Academic Research Experience

University of Pittsburgh

- Graduate Student Researcher — Jan 2020 – present

- **Anhydrous Proton Transport on Graphene-based Materials using Deep Learning** *github.com/siddarthachar/protonConduction_graphanol*
  - 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 for Machine Learning Potentials using Growing Strings**
  - Developed a workflow that uses the growing string method, generative AI, and DFT to build accurate reaction-aware machine learning forcefields.

- **DeepCDP: Deep Learning Charge Density Prediction** *github.com/siddarthachar/deepcdp*
  - 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.
  - Showcased the potential of DeepCDP to track charge centers in complex materials accurately.

- **Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66**
  - 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.

Carnegie Mellon University

➢ Graduate Student Researcher (11-785) Jan 2022 – May 2022

- **Untargeted Adversarial Attacks on Automatic Video Captioning and MyTorch Development** *github.com/RaphaelOlivier/robust_speech*
  - 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.

➢ Graduate Student Researcher Jan 2019 – Dec 2019

- **Evaluation of the degree of rate control via automatic differentiation** *github.com/siddarthachar/dynamicDRC*
  - 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.

R.V. College of Engineering

➢ Undergraduate Research Project Jan 2018 – May 2018

- **Development of Graphene Based Post-Combustion CO2 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

University of Pittsburgh

Teaching Assistantship for Graduate Fundamentals of Reaction Processes (CHE-2201) August 2022-Dec 2022

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

Guest Lecture - Advanced Scientific Visualization (CHE 3460) Nov 2023

University of Pittsburgh

Undergraduate student mentoring August 2020 – present

- Mentored 4 students. All our research work has led to publications (published + under-review).

University of Pittsburgh

President, ChE Graduate Student Association May 2023 – present

- Organized two ChE department research symposium.

Academic Peer-Review (assisted) Jan 2020 – present

Journals: ACS: J. Phys. Chem., J. Chem. Theory Comput, AMI, Appl. Mater. Interfaces, Matt. Lett.; Wiley: ChemPlusChem, Medical Physics Journal; Spinger: EPJP, Nature: Scientific Reports.

Carnegie Mellon University

Social Chair, ChE Graduate Student Association Jan 2019 – Dec 2019

R.V. College of Engineering

Head and Treasurer, RVQuizCorp Aug 2017 – May 2018

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

Presentations

27. **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.
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. 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++, R Programming, MATLAB, Unix shell script (Git)
Computational Chemistry tools: CP2K, VASP, LAMMPS, 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
American Ceramics Society	2021 – 2022