SIDDARTH ACHAR

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Education

University of Pittsburgh, Pittsburgh, PA — **GPA: 3.77/4.00**
Ph.D. in Computational Modeling and Simulation — **Jan 2020 - present**

Carnegie Mellon University, Pittsburgh, PA — **GPA: 3.80/4.00**
Master of Science in Chemical Engineering — **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**

Acemedic Research Expericence

Anhydrous Proton Transport on Graphene-based Materials using Deep Learning — **Dec 2020 - present**
University of Pittsburgh (with Dr. Karl Johnson, Dr. Linfeng Zhang, Dr. Leonardo Bernasconi)
github.com/siddarthachar/protonConduction_graphanol

- Designed a graphane-based material for proton conduction using machine learning (ML) potentials with active deep learning (DL) using the Deep Potential Molecular Dynamics (DeePMD) package.
- Combined quantum mechanics (QM) methods (DFT) with active learning to explore more than 1 million configurations.
- Developed a proton conduction rate equation to specifically study proton hopping.
- Demonstrated that this ML forcefield is capable of understanding charge distribution and simulate proton hopping for multi-protonated systems using LAMMPS for system sizes with more than 10,000 atoms.

Efficiently Trained Deep Learning Potential for Graphane — **Jan 2020 – May 2021**
University of Pittsburgh (with Dr. Karl Johnson, Dr. Linfeng Zhang)

- Generated efficient training data pool of atomic frames using ab-initio molecular dynamics (AIMD) for graphane.
- Designed a neural network using DeePMD to construct a highly accurate DL forcefield for graphane.
- Demonstrated the validity and generality of the DL forcefield by comparing physical properties like stress-strain relations, phonon density of states, thermal fluctuation etc. on LAMMPS with density functional theory (DFT) results.

Study of Ne diffusion in UiO-66 with the first deep learning forcefield for MOFs — **May 2020 – Jan 2021**
University of Pittsburgh (with Dr. Karl Johnson, Dr. Linfeng Zhang, Dr. Leonardo Bernasconi, J. Wardzala)

- Constructed the second neural network forcefield for a metal-organic framework (MOF), UiO-66.
- Developed a unique method to combine DL potentials with classical potentials to compute the diffusion of guest atoms into the MOF in LAMMPS.
- Demonstrated that the ML forcefield is efficient and accurate for the MOF as compared to QM data and experiments.

DeepCDP: Deep Learning Charge Density Prediction — **Sept 2020 - present**
University of Pittsburgh (with Dr. Karl Johnson, Dr. Leonardo Bernasconi)
github.com/siddarthachar/deepcdp

- Built a python package called DeepCDP, which is a framework to build and use ML models for electron density predictions.
- Used the Smooth Overlap of Atomic Positions (SOAP) descriptor technique to generate local atomic environment of grid points in three-dimensional space using QM data.
- Achieved a prediction accuracy of near 100% on test case for complex materials with linear scaling.
- Demonstrated the implementation of DeepCDP for system sizes as large as 10,000 atoms using parallelization.
- Working on integrating this model with LAMMPS for on-the-fly electron density prediction from classical MD as part of the Deepmodeling package (https://github.com/deepmodeling)

Calculation of Degree of Rate control for multistep reactions at steady and unsteady state — **May 2019 - Dec 2019**
Carnegie Mellon University (with Dr. John Kitchin, Yilin Yang)

- Crafted four methods to calculate degree of rate control (DRC) for multi-step catalytic reactions.

- Demonstrated the use of automatic differentiation (AD) tools on python to solve complex rate equations.
- Programmed a python-based used-interface (UI) to automatically calculate steady and unsteady DRCs for any catalytic reaction as per user's input.

Predicting patients with First-Episode Psychosis using sleep spindle from Electroencephalography (EEG) data **Jan 2019 - May 2019**

Carnegie Mellon University (with Dr. John Kitchin), University of Pittsburgh Medical Centre (UPMC)

- Predicted patient's chances as first-episode psychosis (FEP) or healthy-control (HC) with spindle properties from EEG data with logistic regression.
- Performed feature engineering by clustering the human brain into five different sections to increase prediction accuracy.
- Attained an accuracy of 85% by improving the model with cross-validation and hyperparameter optimization.

Development of Graphene Based Post-Combustion CO2 Capture System **Jan 2018 - May 2018**

R.V. College of Engineering (with Dr. Basavaraja R.J.)

- Synthesized lab scale graphene through Hummer's process reducing the production cost by about 30%.
- Devised an experimental plan and selected characterization techniques to test the adsorption capacity of the synthesized graphene.
- Fabricated an adsorption column with an augmented fluid jacket. Adsorption and desorption studies were performed for CO_2 and N_2 to find out the feasibility of graphene as a reusable CO_2 adsorbent. Filed an Indian Patent on the work.

Professional Experience

Computational Material Scientist Intern**, Western Digital.,** *San Jose, CA* **May 2021-Aug 2021**

- Developed several Moment Tensor Potentials using ridge regression that captured inter-diffusion of Ti-$Ge_{20}Se_{80}$.
- Deployed Moment Tensor-drive active learning scheme to generate high temperature training data for bulk crystals that captured one-element and two-element Ti-Ge-Se interactions using QuantumATK package.
- Demonstrated the quality of the potential by comparing equation of state, elastic properties, relaxation trajectories.
- Achieved a speedup of more than 5000 using this potential as compared to DFT methods to simulate Ti-$Ge_{20}Se_{80}$.

Research Intern, **Innovative Nano Materials (INM) Pvt. Ltd.,** *Bangalore, India* **Jan 2017 - Dec 2017**

- Synthesized a coating using MgF_2- TiO_2 composites using sol-gel techniques that increases the transmission of light through solar glass panels by 2%.
- Gained professional lab experience with sol-gels preparation and optical parameter characterization techniques.

Summer Research Fellow**, Saha Institute of Nuclear Physics,** *Kolkata, India* **May 2017 - July 2017**

- Prepared an instrumentation report on the improvement of Secondary Ion Mass Spectroscopy (SIMS)
- Performed research studies on materials to find the elemental composition using SIMS.

Publications *(with hyperlinks)*

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)
6. **Achar, S. K.**, Wardzala, J., Bernasconi, L., Zhang, L., & Johnson, J. K. (2022). A Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66±. Journal of Chemical Theory and Computation (Submitted, under review)
5. Yang, Y., **Achar, S. K,** & Kitchin, J. (2021). Evaluation of the Degree of Rate Control via Automatic Differentiation. AIChE journal (Submitted, under review) (Link)
4. **Achar, S. K.**, Stewart, D. & Schneider, J. (2022). Using machine learning empirical potentials to investigate interdiffusion at metal-chalcogenide alloy interfaces. (Paper in preparation)
3. **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 (Link).
2. Gupta, S., Bonageri, S., **Achar, S. K.,** & Menon, A. (2018). Synthesis of porous graphene powder through improved Hummers' method. In AIP Conference Proceedings (Vol. 1966, No. 1, p. 020014). AIP Publishing LLC (Link).
1. 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).

Conference Presentations

12. **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
11. D. Stewart, **S. Achar**, J. Schneider, Using machine learning empirical potentials to investigate interdiffusion at metal-chalcogenide alloy interfaces. *Intersect (2021),* Barcelona, Spain
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. 2021. Fluid Jacketed Temperature Swing Adsorption System for Carbon Dioxide Capture Using Graphene. India. 202041024611, filed (June 11, 2020), and published (December 17, 2021)

Awards and Sponsors

- Winner 3rd place: *SDLC Partners 2019 Hackathon*, Pittsburgh. 2019
- Awarded *Best Innovative Project in R.V. College of Engineering – 2018*, EDC Development. 2018
- Awarded *Karnataka State Council for Science and Technology (State Government) sponsorship* 2018
- Awarded *Saha Institute of Nuclear Physics Summer Fellowship* 2017

Leadership/Mentorship

- **Mentorship:** Two undergrad Pitt ChemE students during my PhD — August 2020 – present
- **Social Chair** – ChEGSA, Carnegie Mellon University — Jan 2019 – Dec 2019
- **Head and Treasurer** – RVQuizCorp, R.V. College of Engineering — Aug 2017 – May 2018

Skills

Programming Languages: Python (proficient), C++, R Programming, MATLAB Unix shell script, Git
Software for Computational Chemistry: CP2K, VASP, LAMMPS, DeePMD, DPGEN, PyTorch, QuantumATK
Software: Aspen Plus, UniSim, COMSOL Multiphysics, GAMS
HPC related: MPI, OpenMP, pthreads, OpenACC