# SIDDARTH ACHAR

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## Education

**University of Pittsburgh,** Pittsburgh, PA — **GPA: 3.95/4.00**
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**

## Research Projects

**Towards a deep learning potential for anhydrous proton transport** — **Jan 2020 - present**

*University of Pittsburgh (with Dr. Karl Johnson, Dr. Linfeng Zhang)*

- Performed large-scale atomistic simulations for proton transport across functionalized graphane surfaces. Finds application in fuel cells.
- Constructed highly accurate deep learning forcefields with Deep Potential Molecular Dynamics and active learning techniques to efficiently predict energies, stress-strain relations, phonon density of states, velocity auto-correlation function, thermal fluctuation, and other properties of graphane based materials.
- Studied the effect of temperature and system size for training data used in model building.
- Increased the scalability of atoms for predictions from exponential to linear scaling.
- Demonstrated proton hopping across functionalized graphane using a model that was never trained for proton hopping.

**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)*

- Developed four methods to calculate the Degree of Rate Control (DRC) of any multi-step catalytic reaction using automatic differentiation (AD) tools on python.
- Increased complexity and accuracy to compute rate of reaction by solving multiple ODEs with AD.
- Analyzed transient DRC profile for CO oxidation reaction to understand the change in kinetics of the reaction with time. Prior to this, observing transient DRCs were not very prominent.
- Built a python-based user-interface (UI) to automatically calculate steady and unsteady DRCs for any catalytic reaction as per user's input.

**Building highly accurate deep learning forcefields for UiO-66 (MOF)** — **May 2020 - present**

*University of Pittsburgh (with Dr. Karl Johnson, Dr. Linfeng Zhang, Dr. Leonardo Bernasconi), DTRA*

- Deployed active learning techniques to build highly accurate and efficient potentials for large metal-organic-frameworks (UiO-66) that finds applications in breaking down chemical warfare agents.
- Demonstrated that deep learning potential predicts physical properties (like bulk modulus) that are more than 98% accurate compared to experimental results.
- Performed a diffusion study of Neon into UiO-66 using a hybrid potential approach (deep learning + classical) which gave diffusivities of near 100% accuracy to popular classical approaches for the MOF.
- Used hyperparameter optimization to improve the efficiency of the deep learning forcefield.

**A Machine learning approach to predict electronic densities instantly** — **Sept 2020 - present**

*University of Pittsburgh (with Dr. Karl Johnson, Dr. Leonardo Bernasconi)*

- Building a machine learning technique that uses electronic density data on grid space to predict densities for single water molecule during molecular dynamics.
- Feature transformation of grid points in space to input data where symmetry is preserved.
- Accuracy of near 100% on such predictions for data sets with smaller number of atoms.

**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)*

- Used logistic regression to build a model that predicts whether a patient has first-episode psychosis (FEP) or was a healthy-control (HC) in order to replace error prone psychiatric interviews to classify patients.
- Obtained input for the model as the spindle properties of every patient obtained from EEG.
- Performed feature engineering by clustering the human brain into five different sections to increase prediction accuracy.
- Attained testing accuracy of 70% and training 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.

**SDLC Hackathon: Automated process to reduce Hospital readmissions ($17 Billion Problem)** **Sept 2019**

*SDLC Partners, L.P. - Pittsburgh*

- Used UI Path Robotic Process Automation (RPA) tool to automate the process of patient admission in hospital to reduce wait time.
- Applied Machine Learning methods to assist doctors to provide AI aided prescription to patients using their medical history to reduce readmission.
- Developed a patient engagement technology using RPA and Machine Learning to follow up with the patient for after-treatment.

## Professional Experience

**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

- **Achar, S**. K.; Madathil, A. P.; S., Naveen C; Gosh, B.; Phani, A R," Thickness Dependent Optical Properties of Sol-gel based MgF2 – TiO2 Thin Films", (2018, March) In Journal Article Mechanics, Materials Science & Engineering.

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

## Conference Presentations

- **Siddarth Achar**, J Karl Johnson "Towards a deep learning potential for anhydrous proton transport" talk session at American Institute of Chemical Engineers (AIChE) Annual 2020 – (November 2020), San Francisco, CA

- **Siddarth Achar**, Linfeng Zhang, J Karl Johnson "Towards a deep learning potential for anhydrous proton transport" poster presentation at Pittsburgh Quantum Institute 2020 – (October 2020), Pittsburgh, PA.

- **Siddarth Achar**, John R. Kitchin "Calculation of Degree of Rate control for multistep reactions at steady and unsteady state" poster presentation at Pittsburgh-Cleveland Catalysis Society (PCCS – August 2019) Conference, Pittsburgh, PA.

- **Siddarth Achar**, John R. Kitchin “Calculation of Degree of Rate control for multistep reactions at steady and unsteady state” poster presentation at 41st Annual ChEGSA Symposium, CMU – (October 2019), Pittsburgh, PA.

- **Siddarth Achar**, Akhil PM, C.S. Naveen, Baijayanti Ghosh, A.R. Phani “Thickness dependent optical properties of TiO2-MgF2 nanocomposite thin films by using Envelope technique” Oral presentation at the 2nd International Conference on Advances in Materials Science and Technology 2017 (ICAMST – October 2017), VIT Vellore, Tamil Nadu, India.

- Siddhant Gupta, Shrilakshmi Bonageri, **Siddarth Achar**, Basavaraja R.J. “Synthesis of porous graphene powder through improved Hummers’ method” Oral presentation at American Institute of Physics (AIP) Conference (March 2018), Coimbatore, Tamil Nadu, India.

## Awards and Sponsors

- Secured Third place in "SDLC Partners 2019 Hackathon, Pittsburgh" for developing Automated process to reduce Hospital readmissions ($17 Billion Problem). **2019**

- Awarded ‘Best Innovative Project in R.V. College of Engineering - 2018’ by the Entrepreneurial Developmental Cell - R.V. College of Engineering for the "Development of Graphene based Post-Combustion $CO_2$ Capture System". **2018**

- Karnataka State Council for Science and Technology (State Government) sponsor for the project titled "Development of Graphene based Post-Combustion $CO_2$ Capture System". **2018**

## Leadership

- **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 (TensorFlow, scikit-learn), C++, R Programming, Unix shell script, Git
**Software for Computational Chemistry**: CP2K, VASP, LAMMPS, DeePMD, DPGEN
**Software:** Aspen Plus, UniSim, COMSOL Multiphysics, GAMS