

# Positions in Venkat Viswanathan's Group

## Carnegie Mellon University

Our interdisciplinary group works on technologies that can lead to a transition to sustainable energy, supported by several [federal funding agencies and industrial sponsors](#). We actively recruit from MechE, Materials Science, ChemE, Physics and Machine Learning departments at Carnegie Mellon. Students are encouraged to pick the discipline that is the best fit for them. However, if you have a strong interest in **joining our group**, please apply to the **MechE department** and indicate your interest to work in our lab in your research statement. For postdoc positions, directly email me with CV. [Research Website](#)



### Projects for 2019-20 cycle

- **Machine-learning accelerated Energy Materials Discovery and Optimization:** In this project, we will hunt for catalyst systems that efficiently convert CO<sub>2</sub> into carbon-neutral chemicals and fuels. Massive chemical spaces will be evaluated, the search made tractable with the help of machine-learning methods and novel software and hardware acceleration of our group's theoretical catalysis methods. Future work will transfer this framework to another high-dimensional chemical space - designing new electrolyte systems for next-generation batteries.

The project, [described here](#), involves collaboration with Citrine Informatics, Julia Computing and MIT (Alan Edelman), supported by the ARPA-E DIFFERENTIATE program. Work will involve software automation of ab-initio calculations, microkinetic modeling of catalyst reaction pathways, computing acceleration via Julia and GPUs, and machine-learning (global optimization, sequential learning, and neural surrogates for differential equations). (*2-3 PhD/postdoc positions*)

- **Autonomous Electrolyte Discovery:** In collaboration with Jay Whitacre's group, our team is developing robotic experiments that characterize battery electrolytes in an autonomous, high-throughput manner. Our first electrolyte bot, Otto, is online - read more [here](#). (*1 PhD position*)
- **Batteries for Electric Aircraft:** Electrolyte engineering coupled with tortuosity design to achieve high discharge rates, high specific energy. Collaboration with Yet-Ming Chiang. Read more about this project [here](#). (*1 PhD position*)
- **Bayesian Inference Approaches for Cell Testing:** Leveraging our 800 channel battery testing facility, design methods with synergistic computational models enabling 'maximal-information-gain' and parameter estimation to analyze use-case-specific battery performance. Collaboration with Voltaiq. (*2 PhD/postdoc positions*)
- **Machine Learning Accelerated Materials Search:** New materials search typically use methods requiring vast number of DFT calculations. Machine-learned surrogates can rapidly accelerate materials search and enabling inverse material design. (*1 PhD position*)
- **Synthesis Machine Learning:** Data-driven precursor and process conditions from experiments, combined with DFT data to learn synthesis routes for battery materials. (*1 PhD/Postdoc position*)

### Methodological interests

- Computational material design
- Density functional theory simulations
- Phase-field modeling
- Data-driven material discovery
- Machine learning-accelerated design
- High-performance (GPU) computing

### Expected Skill Sets:

- Understanding of thermodynamics and mathematics (numerical methods)
- Strong programming skills (MATLAB/Mathematica/Python/C/C++; Julia incredible plus!)