

Positions in Venkat Viswanathan's group

Carnegie Mellon University

The highly interdisciplinary computational group with close collaborations with experimental groups at MIT, Stanford, UC Berkeley, Caltech, etc., comprises of over ~15 students from Mechanical Engineering, Physics, Chemical Engineering, Materials Science, Engineering Physics, etc. We recruit actively from MechE, ChemE, MSE and Physics departments at Carnegie Mellon. Students are highly encouraged to pick the discipline that is best fit for them. However, if you have strong interest to **join our group**, please apply to the MechE department and indicate your interest to work in our lab in your research statement. [Research Website](#)

Projects for this cycle

- **Next generation batteries for Electric vehicles – Self-forming solid electrolytes:** A combined experimental/computational collaboration between MIT and CMU will investigate electrochemical formation of lithium halide based solid electrolytes, with the goal of enabling and demonstrating self-assembling/self-healing batteries using lithium metal negative electrodes. This will enable batteries with energy densities greater than 400 Wh/kg and overcome their short cycle-life and safety concerns, both associated with dendritic formation. Collaboration with MIT (Yet-Ming Chiang's group). (1-2 PhD/postdoc positions)
- **Electric planes – Li-O₂ batteries for electric aircraft:** We will design novel, ultra-stable electrolytes that are resistant to decomposition so the batteries will last longer, allowing aircraft to extend the distance they can fly. Collaboration with NASA, UC Berkeley and IBM. [Project description](#). (1-2 PhD/postdoc positions)
- **Data-driven discovery – Machine-Learning Unified Synchronous Experimentation:** Our goal is to create an autonomous platform that, based on a set of user-supplied objective functions, boundary conditions, can optimize material properties/performance in real time guided by a ML platform that is informed both by data. (1-2 PhD/postdoc positions)
- **Advanced Battery controls:** The primary objective of this project is to create a new heterogeneous particle battery model for use in control of batteries with strict safety-critical constraints to enable safer and higher energy density batteries. (1 PhD position)
- **Solid electrolytes for Li-ion batteries:** High-throughput data-driven discovery of solid electrolytes that strike trade-offs between mechanical properties, ionic conductivity and electrochemical stability. The project will leverage GPU-accelerated computing. Collaboration with MIT (Yet-Ming Chiang's group). (1-2 PhD positions)
- **Fuel Cells: New Catalysts for Oxygen Reduction Reaction:** We will analyze the use of Pt/adhesion layers formed through ALD to enhance their catalytic activity for oxygen reduction reaction. Collaboration with Stanford (Prinz, Jaramillo group) and Volkswagen. (1 PhD position)

Group's Research Interests

Methodological interests

- Computational material design
- Density functional theory simulations
- Phase-field modeling
- Data-driven material discovery
- Advanced energy Controls
- GPU accelerated computing

Application areas

- Next generation batteries for electric vehicles
- Electric planes
- Fuel cells
- Sustainable chemical and fuel synthesis through electrocatalysis
- Bio-inspired and bio-mimetic materials

Skill sets expected:

- Strong knowledge of thermodynamics, mathematics (numerical methods)
- Strong programming skills (MATLAB, MATHEMATICA, Python)