

# Davidson School of Chemical Engineering welcomes 2017-2018 **New Faculty**



**Dr. Brett Savoie**

*Assistant Professor*

Prior to joining the faculty of the Davidson School of Chemical Engineering, Dr. Brett Savoie earned Bachelor of Science degrees in Chemistry and Physics from Texas A&M University. Dr. Savoie later earned his PhD in Theoretical Chemistry from Northwestern University under the mentorship of Professors Mark Ratner and Tobin Marks for developing theoretical methods to study photovoltaic processes in organic semiconductors.

Most recently, Dr. Savoie worked as a postdoc in the research group of Prof. Thomas Miller at Caltech developing high-throughput methods to screen new polymers and solvents for battery electrolyte applications.

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## The Savoie Research Group

The Savoie group focuses on accelerating the design and characterization of energy-related materials using theoretical methods. Burgeoning computational power and algorithm development have made theoretical characterization and screening essential steps in modern materials development. From first-principles predictions of electronic structure, catalytic activity, and even crystal structure—methods development continues to push the frontier of what material properties can be predicted in advance, thus economizing costly synthesis and optimization efforts.

The Savoie group is building on these advances by developing predictive theoretical methods to characterize transport phenomena in disordered media, including organic semiconductors and membranes. Organic materials are attractive because their electronic, ionic, and mass transport can all be tailored via chemical modifications, but methods need to be developed that can accurately capture the stochastic nature of these materials and shorten the lead-time in developing and deploying new chemistries. The Savoie group is addressing these challenges by (i) developing new simulation methods with the chemical accuracy required to quantitatively describe weak packing-interactions, (ii) developing bottom-up coarse-graining methodologies that can reach the long length and timescales of transport phenomena, and (iii) developing computationally scalable incarnations of these methods that can be used in the high-throughput development of new materials.

Students and postdocs in the Savoie group will learn modern multiscale modeling methodologies, high-performance programming, and hypothesis driven materials design. Interested students and postdocs are welcome to e-mail Dr. Savoie directly or knock on his door to discuss opportunities within the group.

Learn more about the Davidson School of Chemical Engineering at Purdue University at <https://engineering.purdue.edu/ChE>

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