Will minimizing cognitive load improve polymer modeling and make our field more equitable?

Abstract: Sustainably generating energy and manufacturing new composites both depend on engineering the nanostructures of very large systems: Solar panel arrays and airplanes, as examples. Unfortunately, it can be difficult to predict material structure because of experimental or computational limits to observing the required length scales and time scales. Here we focus on strategies for overcoming computational limits to predicting the morphologies in organic materials with applications in power generation and structural composites. We discuss simplified models for overcoming sampling barriers in molecular simulations, and the application of evidence-based instructional practices for overcoming training barriers for new molecular simulators. We find these acceleration schemes enable prediction of some of the largest validated organic photovoltaic and reacting epoxy thermosets to date, and provide an on-ramp for mentors to apply universal design for learning across classroom and lab environments.

Bio: Dr. Jankowski earned his PhD in Chemical Engineering from the University of Michigan in 2012, where he developed computational tools to study the self-assembly of nanoparticles. These tools leveraged graphics processors to accelerate computations and provided insight into systems of both theoretical and practical importance. Dr. Jankowski began focusing on renewable energy generation during his postdoctoral positions at the University of Colorado and the National Renewable Energy Laboratory. At these postdocs, Dr. Jankowski applied techniques he developed during his thesis to understand factors that determine the ordering of molecules in organic solar cells.

Dr. Jankowski also enjoys cycling and an ancient board game (go), and can easily be convinced to discuss how themes of efficiency and combinatorics overlap between these hobbies and his professional interests. His representative animal is an Octopus; ask him about it if you have a few hours to spare.