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Combining modelling, theory, and simulations with experiments for design and structural characterization of soft materials

Monday, 6 June 2022 09:30 (45 minutes)

My research group focuses on development and application of molecular models, liquid state theory, molecular simulation, and machine learning for studying soft macromolecular materials. In this lecture I will share examples of how we develop appropriate molecular models and use them with computational methods to better understand and predict effects of polymer design on the resulting macromolecular material structure and thermodynamics. I will also share experimental work from our collaborators that help us validate our model and computational methods as well as confirm our computational predictions.

Primary author: JAYARAMAN, Arthi (University of Delaware)

Presenter: JAYARAMAN, Arthi (University of Delaware)

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