Joint Condensed Matter and Center for Soft Matter and Biological Physics Seminar

Dr. Michael Salerno

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"Atomistic and Coarse-Grained Polymer Modeling: A Applications at the Army Research Laboratory"

Monday, April 12, 2021

4:00pm – 5:00pm

Virtual Meeting:

Zoom Link: https://virginiatech.zoom.us/j/84822139533

Many fundamental and applied research projects at the Army Research Laboratory (ARL) rely on all-atom molecular dynamics (MD) simulations and also need to extend or couple to adjacent length and timescales. I will discuss two relevant modeling problems that link MD to smaller and larger length scales: First, ab-initio results on molecular photoexcitation are used to model photo responsive molecules in glassy materials. Results from MD simulations show that the dynamics of photoactivated molecules in glassy solids depends critically on local density features. A characteristic power-law wait-time for photoisomerization occurs in samples for densities that vary with photoactive molecule and glass-matrix material. Dynamic behavior is driven by difficult-to-identify local density features, which suggests an opportunity for a machine-learning approach. Second, understanding the shear flow and rheology of polymers like high-molecular-weight polyethylene requires simulations orders of magnitude beyond the lengths and times of atomistic MD.

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