Physical Chemistry Seminar
Virtual
Zoom Link https://udel.zoom.us/j/98093174367
Monday, October 25, 2021, 4pm

How can we unlock the secrets of molecular machines?

How do molecular machines really work? And how can molecular simulations be accelerated to yield reliable insights into such machines? To address the first question, we will explore standard chemical kinetics models of machine function, but with a twist - seeking to find a range of models that can perform a given function. The results point to possible functional and mechanistic heterogeneity of machines beyond what is typically presented in literature cartoons. For the second question, we discuss the “weighted ensemble” method which orchestrates multiple molecular dynamics trajectories and can yield ‘super-parallel’ performance in computing rate constants and mechanism. Recently developed non-equilibrium analysis of trajectory data is shown to be essential.