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Multiscale Dynamics in Soft-Matter Systems: Enzyme Catalysis, Sec-Facilitated Protein Translocation, and Ion-Conduction in Polymers.

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Nature exhibits dynamics that span extraordinary ranges of space and time. In some cases, these dynamical hierarchies are well separated, simplifying their understanding and description. But chemistry and biology are replete with examples of dynamically coupled scales. In this talk, we will discuss the use of high-performance computing and new simulation methods that enable the inclusion of nuclear quantum effects, such as zero point energy and tunneling, in the reaction dynamics of enzymes, as well as coarse-graining strategies to enable minute-timescale simulations of protein targeting to cell membranes and ion-conduction in polymer electrolytes for lithium-ion battery applications.