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Surl-Hee (Shirley) Ahn, Ph.D.

Department of Chemical Engineering
University of California Davis

Bridging timescales between simulations and
catalytic and biological processes

To investigate the structures and dynamics of catalytic and biological processes at an atomic level, computer simulations can be useful since they can serve as a computational microscope. However, electronic structure calculations that are often used to investigate catalytic processes are computationally expensive and cannot reach long timescales as a result. Hence, we have recently developed machine-learned potentials to model gold nanoclusters in zeolite pores or catalysts using molecular dynamics (MD) simulations with density functional theory (DFT) accuracy. Although MD simulations can reach longer timescales compared to DFT, MD simulations also suffer from the timescale barrier between simulations (run using femtosecond time steps) and biological processes (usually milliseconds or longer) by being limited to the slowest motions in the system (e.g., the vibration of bonds). Thus, we have been developing enhanced sampling methods for MD simulations to bridge the timescales and make MD simulations closer to being a true computational microscope that uncovers the fundamental mechanisms of biological processes. In this talk, I will present and discuss both efforts.