# Enabling Long Time-scale Quantum Molecular Dynamics Simulation for 5f-elements

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*Abstract*

5f-element chemistry in solution is very intricate in nature. There is a pressing need to develop molecular dynamics (MD) methods that can describe quantum mechanical behavior, such as bond breaking and forming, at long timescales. Current first-principle MD methods can only reach tens of picoseconds, while classical force fields cannot accurately describe bond breaking and forming.To achieve this goal, we developed semiempirical density functional theory tight-binding (DFTB) parameters for 5f-elements that enable MD simulations at long time scales. Such simulations will be instrumental in understanding the evolution of speciation and reaction mechanisms. In this talk, we will share our recent development on a hybrid model that combines modern machine learning approaches with physics-based methods. We will demonstrate the transferability of this hybrid model on prediction of molecular structural parameters of various molecular clusters and a variety of chemical reaction free energies. Using these parameters, we also demonstrate microsecond-long quantum-MD simulations of nanoparticle systems for complex f-elements, shedding light on their dynamics and kinetics.

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