

New Methods and Models for Condensed Phase Simulation

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I will discuss new theoretical models and extended Lagrangian methods that addresses accuracy and tractability for using atomistic polarizable force fields and linear scaling AIMD. These models and their implementations are opening up new abilities for allowing larger scales of study for molecular simulation with more complex potential energy surfaces. I will highlight a recent application of polarizable models to improve the rate of catalysis by 50X by optimizing electric field environments.