

Adaptive Molecular Dynamics Framework for Viscosity Prediction and Shear-Thinning Analysis of Lubricant Molecules

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Accurate prediction of viscosity and rheological behavior remains challenging due to long relaxation times and significant statistical uncertainty in molecular simulations. In this work, we present an adaptive framework that combines equilibrium and non-equilibrium molecular dynamics simulations to determine viscosity, relaxation times, and shear-thinning behavior of lubricant molecules under elevated pressures.

The workflow integrates automated convergence assessment and uncertainty quantification to establish reliable equilibrium viscosity predictions, while non-equilibrium simulations are used to characterize shear-rate-dependent rheology. Using 2,2,4,4,6,8,8-heptamethylnonane (HMN) as a model system, we demonstrate how relaxation dynamics evolve with pressure and how equilibrium and non-equilibrium viscosity predictions can be unified through master-curve representations.

The proposed approach provides a robust route for transport-property prediction from atomistic simulations and highlights opportunities for future data-driven acceleration of molecular rheology studies on modern HPC platforms.