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Invited talk

Molecular simulations for additives and coatings.

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Molecular simulations are useful tool to investigate the dynamics of tribological surfaces. In this presentation, we demonstrate our extended methods to treat the dynamics of additives in base oils, and surface coatings.

In order to simulate the dynamics of polymer additives, we combine Langevin dynamics for segment motions of polymers, with lattice Boltzmann method for flow of base oils. We succeeded to reproduce the effect of viscosity index improver molecules in both bulk and under confinement. The chemical nature of functional groups on the additive molecules are modeled from quantum simulations.

The other topic is surface coating. In molecular simulation, heat generation and transfer in the sliding interface is very restricted. We introduce novel simulation technique based on smoothed particle hydrodynamics. The surface interactions and frictional oscillation parameters are taken from molecular dynamics simulations. In this simulation, heat generation, plastic deformation, heat transfer in micron scale is reproduced.