Exploring Lubricants: Investigating the Solid-Liquid Interface Using Molecular Simulation

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Lubricants are important for a wide range of processes, but the properties of thin liquid films adsorbed on solid surfaces is not fully understood. Using Monte Carlo molecular simulation techniques, we aim to examine the molecular-level interactions between molecules in the liquid phase and solid substrates. In particular, we are interested in adsorption behavior from multicomponent mixtures of hydrocarbons and mixtures of hydrocarbons with other classes of compounds. Our simulation results show strong evidence of preferential adsorption as well as preferential orientation of molecules to maximize molecule-substrate interactions. For example, constitutional isomers of decane may adopt several orientations in the vicinity of the substrate to increase interactions with both the substrate and the molecular layers that form within the liquid film. The figure shows different arrangements of 2,2-dimethyloctane (green) and 4-propylheptane (red) near the solid interface (vertical blue line) in mixtures with *n*-decane (blue).