Monte Carlo Simulations of Perfluoroalkane-Alkane and Ether-Alkane Mixtures near a Gold Surface

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With rapid technological advances, nanotechnology becomes practical leading our interest to the behavior of lubricants near a solid surface. About 3-6 angstroms from the surface, we observe the formation of the first layer known as the monolayer that retains more solid like properties than a liquid. The behavior of the monolayer is dependent upon the composition mixture in our simulations. Previous research indicates that in a liquid of molecules with the same functional group, the longer chained lubricant will take precedence at the interface due to greater interaction with the surface[1]. In our simulations, we used the Monte Carlo method and TraPPE force field parameters. The simulated mixtures are comprised of alkanes with perfluoroalkanes and with ethers. The behaviors of these mixtures were analyzed using density profiles, mole ratio profiles, heats of adsorption, surface orientation and examining liquid structures near a gold surface.

[1] Castro, M.A., Clarke, S.M., Inaba, A., Arnold, T. & Thomas, K. *J Phys Chem.* **1999**, *5017*, 5023