Simulating Short Ethers Near a Solid Metal (Au) Surface

Selena Watkins and Kelly Anderson
Department of Chemistry, Roanoke College, Salem VA 24153

Prior research has been done to observe orientation and stacking patterns of model lubricant compounds near a solid surface. For example, experimentally, mixtures of linear ethers and alkanes form a solid monolayer exhibiting ideal mixing behavior at the surface interface[1]. Of the existing computational models, linear alkanes have been studied in particular. The effect of the oxygen in linear ethers can be studied by comparison to their alkane analogues of similar size. Using the Monte Carlo method, the effects of ether adsorption near an implicit gold (111) surface with which the molecules can interact are examined. The primary goal of this research is to characterize and quantify the stacking pattern of ethers of varying size in the monolayer that forms on the surface as well as examine monolayer mixing in binary mixtures of diethyl ether with a variety of linear alkanes. Force field parameters were developed such that the oxygen within an ether contributes roughly 43 kJ/mol to the total heat of adsorption on the gold surface, which is in agreement with experimental evidence of ethers adsorbed on platinum[2]. Preliminary work indicates ideal mixing in the adsorbed layer as seen experimentally.

[1] Duim, W.C. & Clarke, S.M. *J Phys Chem.* **2006**, *110*, 23853.
2 Sexton, B.A. & Hughes, A.E. *Surface Sci.* **1984**, *140*, 227.