Monte Carlo simulations of the adsorption from solution of alcohol/alkane mixtures near an explicit platinum surface

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The goal of this project is to study the way that the molecules in an alcohol/alkane mixture interact near an explicit platinum surface. Understanding adsorption is important in many different fields ranging from rheology to catalysts to lubrication. Starting with octanol/alkane mixtures that have been studied before, both experimentally and using molecular simulations with an implicit surface, we hope to validate the parameters that we are using in the simulations. We will examine the way that the size of the molecule affects the ability for that molecule to be adsorbed to the surface, and we will pay special attention to the role that hydrogen bonding from the alcohols plays in the adsorption of molecules to the surface. We plan to explore how the ratio of alcohol size to alkane size impacts the ability for that molecule to be adsorbed to the surface.