Monte Carlo Simulations of Fluorinated Alkanes at an Implicit Gold Surface

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Understanding the solid-liquid interface has applications in the lubricants industry and catalytic chemistry, among others. A useful technique for observing solid-liquid interactions is molecular simulations, where challenging systems and conditions can be simulated and studied with greater ease compared to a wet laboratory. This investigation focuses on mixtures of octane, perfluorooctane, and semi-fluorinated octanes adsorbed at an implicit gold surface using Monte Carlo for Complex Chemical Systems. Initial results indicate less fluorinated species are preferentially adsorbed at the surface.