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Structure and dynamics of fluorinated alkanes on silicon dioxide surfaces MESFIN TSIGE, Southern Illinois University at Carbondale — Despite their great promise in various applications, the structure and dynamics of fluorinated alkanes at interfaces is still an open question. In particular, the knowledge from both theoretical and experimental perspectives is very limited when it comes to understanding the interface between these systems and a solid substrate. Molecular dynamics simulations based on the All Atom OPLS model are used to predict the equilibrium structure and dynamics of short fluorinated alkanes on both amorphous and crystalline silicon dioxide surfaces. In order to understand the effect of layer-layer interaction on the ordering of chains in a given layer, the thickness of the liquid film is increased layer-by-layer from monolayer to multilayers. Results for structural and dynamics of the liquid films near the silicon dioxide surfaces will be presented.

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