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Molecular Simulation of Oligomeric Nanofilms Confined Between Iron and Iron Oxide Surfaces DAVID RIGBY, Accelrys, Inc, RAJESH KHARE, University of Wisconsin, Madison, DAVID RIGBY COLLABORATION, RAJESH KHARE COLLABORATION — The past several years have witnessed significant advances in areas of molecular simulation of relevance to the study of confined oligomeric nanofilms. Two noteworthy advances include developments in classical force fields, which promise to make accurate predictions of physical properties, such as equation of state behavior under a wide range of conditions of temperature and pressure, accessible via simulation, and developments in procedures for modeling the behavior of films with nanoscopic dimensions under shear and at equilibrium . In this work, we report on recent calculations in which we have combined these two developments to perform realistic simulations of oligomers confined between iron and iron oxide (as FeO) surfaces. We begin by presenting the results of validation data for the bulk substances of interest – including alkanes, alcohols and bulk metal oxide, before comparing the structure and shear behavior of films consisting either of pure alkanes, or hydroxyl terminated chains. Finally, we examine the effect of enhancing the substrate interaction by use of molecules with additional hydroxyl groups.

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