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Interfacial Properties of Semifluorinated Alkane Diblock Copolymers FLINT PIERCE, DVORA PERAHIA, Department of Chemistry Clemson University, MESFIN TSIGE, Department of Physics Southern Illinois University, OLEG BORODIN, Department of Materials Science and Engineering and Department of Chemical and Fuels Engineering University of Utah, GARY GREST, Sandia National Laboratory — The surface interaction of semifluorinated alkane diblock (SFAs) copolymers with water and normal alkanes are studied using explicit atom molecular dynamics (MD) simulations. At the diblock/air interface, the surface is dominated by fluorinated groups as a result of their low surface tension, and these groups reside at the interface for longer periods of time than the hydrogenated groups. Fluorinating even a single end group on an otherwise hydrogenated chain results in low surface tensions, close to that of perfluoroalkanes and far from normal alkanes. For the interface with water, results for the rate of water uptake by alkanes, perfluoroalkanes, and SFAs will be presented. Additionally, we report the interfacial surface tensions and equilibrium density profiles for these samples, focusing on the prevalence of fluorinated and hydrogenated segments at each interface. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04- 94AL85000.

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