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Interaction of Self-Assembled Monolayers of Oligo(ethylene glycol)-Terminated Alkanethiols with Water studied by Vibrational Sum Frequency Generation (VSFG) JOERG FICK, RONGYAO WANG, SASCHA HERRWERTH, WOLFGANG ECK, MICHAEL HIMMELHAUS, MICHAEL GRUNZE, APPL. PHYS. CHEMISTRY, UNIV. HEIDELBERG TEAM — Conformational changes in oligo(ethylene glycol)-terminated (OEG) self-assembled monolayers (SAMs) have been a topic of interest in recent years because of their crucial role for the protein repulsion properties of these SAMs. In our study, VSFG was used to investigate the conformational changes of hexa(ethylene glycol) (EG6OMe)terminated SAMs on gold, when exposing these films successively to liquid water, to the ambient, and to vacuum. The spectra show that the OEG films in water contact are in a disordered, solvated state. This disorder is partially maintained after removing the samples from direct water contact. It is not until evacuation of the samples that the molecules revert to their original, ordered state. Our study is the first to give experimental evidence for the presence of bound water molecules in the SAM, thereby supporting recent ab initio calculations and Monte Carlo simulations.

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