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Aqueous Surfactant Self-Assembly at Solid-Liquid Interfaces ALBERTO STRIOLO, NAGE RAJESH TUMMALA, CAMILLE GUTIG, BRIAN GRADY, University of Oklahoma — We conducted a series of experimental adsorption isotherms for aqueous non-ionic (C12E6) and ionic (CTAB) surfactants on Au (hydrophobic), SiO₂ (partially hydrophilic), and Al₂O₃ (hydrophilic) surfaces at room temperature. The amount of surfactant adsorbed per unit surface area was measured as a function of the surfactant bulk concentration by means of a Quartz Crystal Microbalance. To assess the equilibrium adsorbed structures we conducted all-atom molecular dynamics (MD) simulations for surfactants at the water-graphite and water-SiO₂ interfaces. The results not only provide a molecular interpretation for the experimental data, but also allow us to identify the driving forces responsible for the surfactant self-assembly. For example, our MD calculations predict that SDS form hemicylindrical structures at water-graphite interfaces, in agreement with solution AFM studies (Wanless and Ducker, JPC 100, 1996, 3207). By conducting test simulations for SDS-like surfactants in which we suppressed surfactant head – counter ion electrostatic interactions we proved that the hemicylindrical structure forms because of the condensation of counter ions near the hydrophilic SDS surfactant heads.

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