

Abstract Submitted
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Orientation of surfactant self-assembled aggregates on graphite

MARIA SAMMALKORPI, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA, ANTTI-PEKKA HYNNINEN, ATHANASSIOS Z. PANAGIOTOPOULOS, Department of Chemical Engineering, Princeton University, Princeton, New Jersey 08544, USA, MIKKO HAATAJA, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA — Micellar aggregates on surfaces can provide a self-healing corrosion protection or lubrication layer. It has been observed experimentally that on a single crystal surface this layer often consists of oriented hemi-cylindrical micelles which are aligned with the underlying crystal lattice (“orientation effect”). A key feature of this self-assembly process is the interplay between detergent–detergent and detergent–surface interactions. Since the dimensions of the detergent molecules and the unit cell of the surface are typically quite different, the origins of this orientation effect remain unclear. Here we address the question and present the results of Molecular Dynamics simulations of sodium dodecyl sulfate (SDS) self-aggregation on graphite. We employ both single-molecule and multi-molecule simulations of SDS to unravel the origins of the orientation effect. We report that the underlying graphite surface is sufficient to impose orientational bias on individual SDS molecules diffusing on the surface. This produces collective effects that give rise to the oriented hemi-micelles.

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