

**Atom-scale structure, dynamics and energetics of alkanethiol bilayers as nanostructure-directing agents**

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Many emerging applications of nanostructures involve organic molecules chemi- or physisorbed at their surfaces. Lamellar metal-oxides have applications ranging from energy-storage, electrocatalysis, the harnessing of electrochromic and photoelectrochromic properties, application in display devices, photovoltaics, to novel energy-conversion systems, proton-pump electrodes, sensors, or chemiresistive 'artificial nose' detectors. As the nanostructures approach the molecular scale, the conformation of molecules adsorbed at their surfaces will inevitably be influenced by the nanoscale geometry. The motivation for this work stems from the profound attention that non-carbonaceous nanostructures are currently receiving. One-dimensional nanomaterials, such as nanotubes, nanowires, and nanobelts or nanoribbons have attracted considerable attention in the past decade because of their novel and useful physical properties such as semiconductivity and acting as a transparent metal in its doped state, leading to immediate applications. Besides the use of 1D nanostructures in electronics as functional components and interconnects in dense, high-speed circuits, they also have numerous applications among others in the design of ultra-small sensors, optical elements for optoelectronics, non-linear optical converters and information storage devices. The objective of the work outlined in this proposal is to use all-atom MD simulations to clarify and understand the role of organic surfactant molecules on polymorphisms of metal-oxide lamellar nanostructures. Previous structural models for bending, and in some cases (depending on the nature of organic structure-directing agent) nanotube formation, are too simple and consistently reiterated a condensation mechanism and eventual scrolling; the reason behind layer scrolling, bending and breakage has proven elusive for these technologically important materials. The layered turbostratic structure of metal-oxide nanofibers, when preserved, could provide a new organic templated-synthesis route for the fabrication of thin-film layered nanostructures. The advantage of template-based growth methods is the ability of fabricating unidirectionally aligned and uniformly sized nanostructured arrays of a variety of materials. The knowledge of the atomic arrangements in these crystalline compounds is a key point for the understanding of the chemical and physical properties which could even range to controlled nanocantilever action and artificial muscles. We want to study the atom-scale mechanism behind laminar curvature in a SAM-intercalated system, by explaining the influence of synthesis parameters (specifically the organic molecule and temperature), prerequisite for the (eventual) elucidation of the mechanism of layer scrolling to form the tubular shape.