

Abstract Submitted
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Morphology of benzene and pentacene self-assembled monolayers and gold-molecule-gold junctions.¹ LEONIDAS TSETSERIS, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN, and Solid State Division, Oak Ridge National Lab, Oak Ridge, TN — The structural properties of self-assembled monolayers of organic molecules or nanostructures on metallic or semiconductor surfaces are critical in determining the electronic and transport properties of such configurations. Here we report results obtained by first-principles density-functional calculations on a number of systems. We first describe the morphology of benzene-dithiolate films on gold surfaces. Special emphasis is given on the behavior of the ultrathin film during the deposition of the second electrode, particularly on the kinetics of cleavage of hydrogen and formation of covalent S-Au bonds. We also discuss the work of Xu and Tao² on formation of molecular junctions, and we analyze the distinct structural phases that can relate to quantum conductance observed in these experiments. Finally, we present results on the growth of pentacene films on Si and SiO₂ surfaces, examining the possibility of forming chemisorbed structures.

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²B. Xu and N. J. Tao, *Science* **301**, 1221 (2003)

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