

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Design Principles Incorporating Surface Dynamics for Creating Ordered Organic Nanostructures on Si and SiC Dimerized Surfaces via Car-Parrinello Molecular Dynamics** ROBIN HAYES, MARK TUCKERMAN, New York University — Self-assembled organic nanostructures on Si-type semiconducting surfaces promise to impact nanoelectronics, sensors, and nanolithography. Experimentalists have long exploited cycloaddition reactions between small conjugated molecules and Si surface dimers, but with limited success in creating well-ordered structures. Cycloaddition of 1,3-cyclohexadiene (CHD) to the Si(100)-2x1 surface provides a rich test case to explore the role surface dynamics plays in adduct formation because of the variety of bonding motifs and discrepancy of the product distribution with thermodynamic predictions. Car-Parrinello molecular dynamic simulations reveal that the local surface environment, including dimer tilt angle and dimer flipping, matters. CHD often travels over several dimers before forming an adduct by a two step process. First the C=C reacts with a “down” Si. The intermediate can persist for over 4 ps and can cause nearby dimers to flip, allowing CHD to complete the reaction with any of the adjacent Si. Thereby, accounting for most of the experimental product distribution. Previously formed adducts protect Si within a 5.5 Å radius and direct the surface exploration of unbound CHD. These principles are tested on reactions between 1,3-CHD and the closely related 3C-SiC(001)-3x2 surface.

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Date submitted: 17 Nov 2006

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