

[SS-09]

Self-assembled molecular arrays on semiconductor surfaces

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The recent demonstration of self-assembled organic wires and films on the Si(001) surface has received widespread attention because of the possibility of combining the wide range of functionality of organic molecules with the existing Si-based infrastructure [1,2]. Ordered arrays of organic molecules in such a hybrid organic-silicon system can be utilized for various technological applications such as optical devices, chemical sensors, and molecular electronic devices. In this talk I present first-principles density-functional theory calculations for various hybrid organic-silicon systems including one-dimensional (1D) molecular wires, two-dimensional (2D) monolayer films as well as 1D Si dangling-bond wire. For 1D molecular wires we study a self-directed growth of molecular line on an H-terminated Si(001) surface. The resulting molecular line which provides electronic channels for charge transport could be used for 1D molecular nanoconductors. For formation of 2D monolayer films we study the reaction of unsaturated hydrocarbons with the (001) surfaces of Si, Ge, and diamond. The calculated reaction paths of unsaturated hydrocarbons on the three (001) surfaces show subtle differences of adsorption kinetics, predicting different orders of the reactivity among each other. Especially, the reaction of acetylenic (containing the triple C-C bond) and olefinic (containing the double C-C bond) molecules with Si(001) occurs with a small energy barrier through a low-symmetry precursor state formed by the attraction between the pi bond of unsaturated hydrocarbons and the electron-deficient down atom of the Si dimer. Our results provide a theoretical basis for the interpretation of recent various experimental data for the adsorption of organic molecules on Si(001), Ge(001), and diamond(001) surfaces.

[References]

- [1] R. A. Wolkow, *Annu. Rev. Phys. Chem.* 50, pp 413 (1999).
- [2] G. P. Lopinski, D. D. M. Wayner, and R. A. Wolkow, *Nature*, 406, pp 48 (2000).