Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Coverage dependence of 1-propanol adsorption on the Si(001) surface and fragmentation dynamics JIAN-GE ZHOU, FRANK HAGELBERG, Jackson State University — The chemisorption of organic molecules on silicon surfaces is a highly topical subject of current research, both experimental and computational. This interest may be ascribed to both the fundamental nature of this problem, involving the interaction between finite units and periodic substrates, but also to its relevance to various areas of recent technology, such as insulator films, nanolithography, chemical and biological sensors, and molecular electronics. The organic layers are formed by depositing organic compounds on the semiconductor surface. In order to optimize this process, the understanding of the interaction between the surface and the organic species is crucial. The geometric, electronic, energetic, and dynamic properties of 1-propanol absorbed on the Si(001)-(2x1) surface are studied from first principles by use of a slab approach. The 1-propanol molecule initially interacts with the Si surface through formation of a dative bond, subsequently the physisorbed 1-propanol molecule reacts with the surface by cleavage of the O-H bond, and the Si(001)-(2x1) surface undergoes further reconstruction as a result of the adsorption of the organic species. The band structure and density of states (DOS) are first analyzed for this system. The band gap of the Si-1-propanol film increases as the coverage level is enhanced. Good agreement is found with available experimental data.

Jian-Ge Zhou
Jackson State University

Date submitted: 16 Jan 2006 Electronic form version 1.4