Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Organic coverage of the silicon (100) surface: first-principles calculations GIOVANNI CANTELE, CNR-INFM and University of Napoli "Federico II", IVO BORRIELLO, University of Napoli "Federico II", DOMENICO NINNO, CNR-INFM and University of Napoli "Federico II" — Interfacing semiconductor surfaces with organic molecule adsorbates is one of the most challenging aspects of the modern surface and interface engineering. Controlled and periodic surface coverage can have important implications in lots of technological applications, such as molecular sensing, molecular electronics, etc. One of the widely investigated surfaces is the silicon <100>. Such a surface shows a periodic arrangement of silicon dimers (induced by reconstruction) whose bonding has been extensively debated. It turns out that its properties are similar to those of a double carbon-carbon bond, and it is therefore suitable for attaching organic molecules, especially those containing a double bond. In this study we theoretically investigate from first principles the adsorption of ethylene, cyclopentene and a class of its derivatives on the Si <100> surface, discussing the implications in tailoring the surface properties, such as the electron affinity and work function. Each molecular adsorbate induces a dipole layer on the surface, whose magnitude depends on the considered molecular species. Our findings demonstrate that, for this class of systems, it is not enough the knowledge of the isolated molecule properties for predicting the properties of the surface-adsorbate complex.

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Date submitted: 27 Nov 2007 Electronic form version 1.4