III. SEMICONDUCTOR SURFACE STUDIES

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1. ELECTRONIC STRUCTURE OF HOMOPOLAR AND HETEROPOLAR SEMICONDUCTING SURFACES

Joint Services Electronics Program (Contract DAAG29-78-C-0020)

John D. Joannopoulos, Eugene Mele

We are continuing our studies of the intrinsic and extrinsic surface states at surfaces of Group IV, III-V, and II-VI semiconductors. In this work we are using a theorem we developed which reduces the semi-infinite surface system to an effective one-dimensional problem that can be solved with transfer matrix techniques. The electrons are studied with realistic tight-binding Hamiltonians which provide an attractive and physical real-space description of the states.

Specifically, we have been studying the nature of semiconductor metal interfaces. We have introduced a new ionicity scale that accounts for the remarkable covalent-to-ionic behavior of Schottky barriers with metal work functions. We are currently investigating the effects of submonolayer and monolayer coverages on Schottky-barrier functions.

2. SURFACE PHONONS IN BONDED SOLIDS

U. S. Navy – Office of Naval Research (Contract N00014-77-C-0132)

John D. Joannopoulos, Robert B. Laughlin

We are continuing our studies of the nature of surface phonons in bonded solids. Particular attention is focused on disordered systems with large internal voids. These materials (e.g., SiO_2) have a massive internal surface area that makes them amenable to studies with conventional phonon probes (e.g., Raman, infrared, etc.). The theory involves treating the system in terms of Bethe lattices which are attached to surface atoms in various ways and describing the potential energy of the atoms in terms of force-constant models. Local densities of states along with theoretical Raman, IR, and neutron cross sections have been calculated. These response functions have been helpful in unraveling many of the puzzling experimental measurements on these materials. We are currently involved in investigating excitations at interfaces between Si and SiO_2.