III. SEMICONDUCTOR SURFACE STUDIES

Academic and Research Staff

Prof. J.D. Joannopoulos
Dr. R.B. Laughlin
Dr. Y-M. Wang

Graduate Students

E.M. Kunoff
D-H. T. Lee
W.R. Pollard

1. EXCITATIONS AT SURFACES AND INTERFACES OF SOLIDS

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

John D. Joannopoulos, Yi-Ming Wang, D-H. Tom Lee

We have developed techniques which allow us to calculate the elementary excitations of crystalline surfaces exactly within a localized orbital approach. This approach provides an attractive and physical real-space description of the states of the system.

Specifically, we have developed a microscopic theory of Fermi-level pinning and Schottky-barrier formation in metal-semiconductor junctions for submonolayer and monolayer metal surfaces. The theory explains how the Schottky barrier can be formed at such low coverage and describes novel exchange reactions at the surface of the semiconductor.

In addition, we have studied the effects of cleavage steps at surfaces and find a very strong correlation between the density of such steps and the unusual band-bending behavior that is observed experimentally depending on the nature of the surface.

We are currently investigating the electronic states at wurtzite surfaces and the effects of core-excitons on surface-state properties.

(III. SEMICONDUCTOR SURFACE STUDIES)

2. SURFACE AND DEFECT EXCITATIONS IN COVALENTLY BONDED SOLIDS

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

John D. Joannopoulos, Robert B. Laughlin, Estelle M. Kunoff

We have developed a theoretical formalism that will enable us to study the electronic states at disordered Si-SiO_2 interfaces. In particular, we have concentrated on developing a realistic tight-binding model to describe accurately the electronic states and wave functions in bulk crystalline and amorphous SiO_2. We find that most of the features of SiO_2 are insensitive to topology and are thus universal among all allotropes in which the integrity of the SiO_4 tetrahedron is preserved. A remarkable effect of this universality is a dipole selection rule forbidding the first optical transitions. We are currently investigating the properties of Si-SiO_2 interfaces.