III. SEMICONDUCTOR SURFACE STUDIES

Academic Research Staff

Prof. John D. Joannopoulos

Graduate Students

Robert B. Laughlin
Eugene Mele
William B. Pollard

1. ELECTRONIC STRUCTURE OF HOMOPOLAR AND HETEROPOLAR SEMICONDUCTING SURFACES

Joint Services Electronics Program (Contract DAAB07-76-C-1400)

John D. Joannopoulos

We are interested in a theoretical investigation of the electronic states at the surfaces of Group IV, III-V, and II-VI semiconductors. Because of the lack of complete periodicity when dealing with a "semi-infinite" surface system, we are faced with severe obstacles in making a realistic theoretical investigation. Nevertheless, we have recently constructed a theorem demonstrating that any semi-infinite surface system that can be described by a Hamiltonian of finite range can be reduced to an effective one-dimensional problem that can be solved with transfer matrix techniques.

We have used this theorem with realistic tight-binding Hamiltonians to study the effects of surface atom relaxations in the heteropolar compounds. Our results show that the unfilled surface states are very sensitive to the nature of the Hamiltonian that is used. Given a relaxation, these states will move out of the gap if the cation/anion p-like character of the bulk conduction bands is large enough. In this way the behavior of states at the surface is directly related to properties of the bulk system. It is therefore of paramount importance for theoretical models to describe certain features of the bulk system correctly.

At present, we are investigating the effects of oxygen adsorption on the surface of GaAs. The O interaction integrals can be obtained from studies of molecular O_2 and GeO_2. In this way we hope to determine where the oxygen is adsorbed, and whether it is adsorbed as O or O_2 or in some type of mixed bridging configuration.