III. SEMICONDUCTOR SURFACE STUDIES

Academic Research Staff

Prof. John D. Joannopoulos

Graduate Students

Eugene Mele

A. ELECTRONIC STRUCTURE OF HOMOPOLAR AND HETEROPOLAR SEMICONDUCTING SURFACES

JSEP

Joint Services Electronics Program (Contract DAAB07-75-C-1346)

John D. Joannopoulos

We are interested in 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. Our approach has been to replace the ideal semi-infinite system with an infinite "slab" system. With the use of such a system, our results on GaAs predict new surface states in the antisymmetric gap of the (110) surface. The nature, localization, and character of these states has been determined.

We have also developed a new method, a Gaussian relaxation method, which makes tractable the study of finite but very large systems. It is a local formalism based on an effective Green's function from which local density of states and charge densities can be obtained. With the use of realistic tight-binding Hamiltonians, preliminary results on vacancies in Ge have yielded densities of states and charge densities comparable to those for Si obtained by using self-consistent pseudo-potential techniques. The Gaussian relaxation method should be very useful for studying surface systems with large surface reconstructions, for example, Si (7 × 7), Ge (2 × 8).

Finally, we have 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 matrix transform techniques. This theorem is being used to study relaxation effects in GaAs (110) and the effects of O_2.

JSEP