2. Semiconductor Surface Studies

Academic and Research Staff

Prof. J.D. Joannopoulos, Dr. J. Ihm

Graduate Students

Y. Bar-Yam, D.-H. T. Lee, D. Stone

2.1 Excitations at Surfaces and Interfaces of Solids

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John D. Joannopoulos, Dung-Hai T. Lee, David L. Stone

Understanding the properties of surfaces of solids and the interactions of atoms and molecules with surfaces has been of extreme importance, both from technological and academic points of view. The recent advent of ultrahigh vacuum technology has made microscopic studies of well-characterized surface systems possible. The way the atoms move to reduce the energy of the surface, the number of layers of atoms involved in this reduction, the electronic and vibrational states that result from this movement, and the final symmetry of surface layer are all of utmost importance in arriving at a fundamental and microscopic understanding of the nature of clean surfaces, chemisorption processes, and the initial stages of interface formation.

The theoretical problems associated with these systems are quite complex. We are, however, currently in the forefront of being able to solve for the properties of real surface systems (rather than simple mathematical models). In particular, we have recently developed a new theoretical scheme (faster by an order of magnitude than currently available techniques) which enables us to realistically calculate the electronic and vibrational states at clean and chemisorbed surfaces. In this way, we can study surfaces with large and complex surface unit cells, including certain surfaces of Si, GaAs, SiC, and ZnO.

Actually, one of the most difficult and fundamental problems in surface studies, both from the experimental and theoretical points of view, is the determination of the precise positions of the atoms on a surface. Currently, there are many surface geometries, even for elemental surfaces, that remain extremely controversial. We have begun to develop a method of calculating the total ground-state energy of a surface system from "first principles" so that we may be able to provide accurate theoretical predictions of surface geometries. This will include both clean and chemisorbed surface geometries.

2.2 Surface and Defect Excitations in Covalently Bonded Solids

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John D. Joannopoulos, Jisoon Ihm, Yanaer Bar-Yam

Our work in this area is directed along two thrusts. The first concerns studies of possible defects and disorder in solids from a realistic, microscopic point of view where one is interested in the electronic and vibrational properties of specific arrangements of "real" atoms.

For example, the recent discovery of amorphous Si materials that can be doped and the subsequent construction of solar cells has inspired an enormous amount of research activity attempting to characterize and understand the fundamental properties of these materials. Currently, there is great interest in understanding the structure of silicon-fluorine alloys which seem to make the best devices. We have developed a theory of the vibrational excitations of such systems by studying specific possible Si-F bonding conformations in the system. We have also formulated a theory of the Raman and IR activity of these materials and have made predictions concerning the relationship between the geometric structure of the material and its vibrational excitations.

The second thrust involves studies directed more along a statistical-mechanical approach where one is investigating disorder and localization using simple-model Hamiltonians to represent "real" systems. For example, currently there is great interest in understanding the nature of the resistance of very thin wires at very low temperatures. If the disorder in the wires is made large enough, the theoretical speculation is that one will measure huge fluctuations in the resistance. In particular, we have performed analytical calculations of the arithmetic and geometric means of the resistance for a simple-model Hamiltonian. The results indicate quite clearly that the arithmetic mean is not representative of the distribution, but the geometric mean is. It is found to grow essentially exponentially with the length of the sample.