2. Semiconductor Surface Studies

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2.1 Excitations at Surfaces and Interfaces of Solids

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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 the 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. Actually, one of the most difficult and fundamental problems in surface studies, both from the experimental and theoretical points of view, is simply 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.

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 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. Recent results of metal atoms deposited on a semiconductor surface look very promising. The first total energy map for an interacting atom-surface system has been obtained. The map clearly illustrates possible chemisorption sites as well as specific migration or diffusion channels.

Presently, we are attempting to combine the results of microscopic total energy calculations with the renormalization group techniques, developed in statistical mechanics, in order to study structural phase transitions at finite temperatures. If successful, this will provide an "ab-initio" framework for studying phase transitions and critical phenomena in solid systems.