Chapter 3

SOLID SURFACES

All solids are finite in size and have to terminate on all sides. Exposed surfaces of a solid crystal have distinctive structures and properties that may vary significantly with how the surfaces are prepared. Surface preparation is an art form and an important field of study in its own right. When adequately prepared, surfaces of crystalline solids can accommodate various chemical and physical processes important for applications. Numerous long-standing scientific journals exist that are dedicated entirely to the science and applications of surfaces.[1] Examples of how surface scientists have been able to control and manipulate the structures and properties of the surfaces for applications have been astonishing to witness. The richness and maturity of surface science notwithstanding, our own discussion of the surfaces will cover only a small part: the determination and explanation of the energy band position with respect to the vacuum level at a crystal surface. Properties of the surface that are related to the energy level alignment problem will be examined. How the electronic states are formed at clean or adsorbate-covered surfaces, what determines the placement of the energy bands of the crystal with respect to the vacuum level, and how the surface potentials and dipoles may be modeled, etc. will be the focus of our discussion. A surface may be viewed as the interface between a "crystal" and "vacuum". As such, the alignment of the crystal bands with respect to the vacuum at a surface perhaps offers the simplest example to examine the general problem of interface band alignment. Since vacuum has no structure and is obviously "simple", one may suspect that the energy level alignment condition for the surface, such as the WF of a metal, is easier to analyze and more accurate to predict than that at interfaces between two solids. This is not the case, however. The replacement of material beyond a plane of a crystal with vacuum to create a surface represents a more severe