

III. SEMICONDUCTOR SURFACE STUDIES

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1. ELECTRONIC STRUCTURE OF HOMOPOLAR AND HETEROPOLAR SEMICONDUCTING SURFACES

JSEP

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Our objectives constitute a theoretical investigation of the electronic states at the surfaces of Group IV, III-V, and II-VI semiconductors. Specifically, we have been studying the existence and character of surface states by examining the complete valence bands for unrelaxed and unreconstructed surfaces. Our approach has been to use simple tight-binding Hamiltonians to study two types of surface systems. The structure of these systems is that of a diamond or a zinc blende that is respectively semiinfinite or finite in one direction, and infinite and periodic in the two other directions. Preliminary results show the presence of new surface states in the antisymmetric gap of III-V and II-VI surfaces.

The effects of relaxation, reconstruction, and adsorbates are also being studied. Surfaces with steplike features will be examined to determine their effects on the electronic properties of the surface.

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