III. SEMICONDUCTOR SURFACE STUDIES

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1. EXCITATIONS AT SURFACES AND INTERFACES OF SOLIDS

Joint Services Electronics Program (Contracts DAAG29-78-C-0020 and DAAG29-80-C-0104)

John D. Joannopoulos, Yi-Ming Wang, Dong-Hai T. Lee

We are continuing our studies of the elementary excitations at surfaces and interfaces of semiconducting systems. In particular, we have recently developed a successful theory of surface core-excitons that explains the unusual binding energies measured experimentally. Moreover, a universal limit to the binding energy is predicted that depends only on the nature of the atoms surrounding the excitonic atom.

We are also engaged in an investigation of the properties of compound wurtzite surfaces. This includes a study of both the unique dimerlike and chainlike nonpolar surfaces. Preliminary results on ZnO indicate important differences in the nature of the empty surface states at these surfaces. In addition, bona fide surface states are predicted to exist in the d-like valence states of this material.

2. SURFACE AND DEFECT EXCITATIONS IN COVALENTLY BONDED SOLIDS

U.S. Navy — Office of Naval Research (Contract N00014-77-C-0132)

John D. Joannopoulos, Estelle M. Kunoff

A theory of the Si-SiO_2 interface based on recent experimental findings for silicon surfaces and their oxidation has been developed. We find that a simple local-orbital picture can simultaneously describe silicon, its oxidation, and the

Si-SiO_2 interface. Calculations have been performed which show that interface states do not arise simply from the presence of a boundary. We find that band tailing at the interface is due primarily to strain rather than to charged centers, and predict that dangling bands at the interface should give rise to an inhomogeneously broadened discrete level at midgap.