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Simulation of Non-contact Atomic Force Microscopy for Structural Analysis JAMES CHELIKOWSKY, TZU-LIANG CHAN, University of Texas at Austin, C.Z. WANG, KAI-MING HO, Ames Laboratory of US DOE, Iowa State University — A powerful probe of materials centers on the use of atomic force microscopy (AFM). However, an analysis of AFM images can be complex and problematic. We will present an efficient scheme to simulate non-contact AFM images by employing a first-principles self-consistent potential from the sample as the essential input. This scheme does not require an explicit modeling of the AFM tip. Our method will be illustrated by applying it to various types of semiconductor surfaces including Si(111) (7x7), TiO2 (110) (1x1), Ag/Si(111)- ($\sqrt{3} \times \sqrt{3}$) R30^o and Ge/Si(105) (1x2) surfaces. We obtain good agreement with experimental results and previous theoretical studies by using this scheme. The method can quickly and efficiently aid in identifying different models for surface structures.

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