Abstract Submitted
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Efficient first-principles simulation of non-contact atomic force microscopy for structural analysis[1] JAMES CHELIKOWSKY, TZU-LIANG CHAN, University of Texas at Austin, CAI-ZHUANG WANG, Ames Laboratory-U.S. DOE , KAI-MING HO, Iowa State University — Non-contact atomic force microscopy (nc-AFM) has made significant advances that have allowed one to image a surface at atomic resolution. However, first-principles simulations of nc-AFM images remain a challenge because they involve calculations of the sample together with an atomic model of the AFM tip. We propose an efficient scheme to simulate nc-AFM images by using a first-principles self-consistent potential from the sample as input and without explicit modeling of the AFM tip. Our method is applied to various types of semiconductor surfaces including Si(111) (7×7), $TiO_2(110)$ $(1{\times}1)$, Ag/Si(111)-$(\sqrt{3} \times \sqrt{3})R30^\circ$ and Ge/Si(105) (1×2) surfaces. Our method takes into account electronic effects of the tip-sample interaction, which are important for predicting the bright spot positions and the contrast change with AFM tip height. In addition, we obtain good agreement with experimental results and previous theoretical studies.

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