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Simulated non-contact atomic force microscopy based on real space pseudopotentials and density functional theory MINJUNG KIM, JAMES CHELIKOWSKY, The University of Texas at Austin — Non-contact atomic force microscopy (nc-AFM) is a commonly used technique in surface and nano science owing to its high-resolution and ease of implementation. Theoretical simulations of nc-AFM have been able to facilitate the interpretation of experimental images. However, first-principles AFM simulations can be computationally intensive and problematic if the morphology of the AFM tip is unknown. We introduce an efficient simulation method that does not include an explicit morphology for the tip as suggested by Chan and coworkers.[1] Our method is based on a real space implementation of pseudopotentials constructed using density functional theory. We illustrate the method by simulating nc-AFM images for binary semiconducting materials, *e.g.*, the GaAs(110) surface, and compare our results to previously performed first principles simulations as well as experimental data.

[1]T. -L. Chan, C. Z. Wang, K. M. Ho, and James R. Chelikowsky, *Phys. Rev. Lett.* **102**, 176101 (2009)

Minjung Kim
The University of Texas at Austin

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