

Abstract Submitted  
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**Simulating contrast inversion in atomic force microscopy imaging with real-space pseudopotentials**<sup>1</sup> ALEX LEE, YUKI SAKAI, JAMES CHELIKOWSKY, The University of Texas at Austin — Atomic force microscopy measurements have reported contrast inversions for systems such as Cu<sub>2</sub>N and graphene that can hamper image interpretation and characterization. Here, we apply a simulation method based on *ab initio* real-space pseudopotentials to gain an understanding of the tip-sample interactions that influence the inversion. We find that chemically reactive tips induce an attractive binding force that results in the contrast inversion. The inversion is tip height dependent and not observed when using less reactive CO-functionalized tips.

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