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Simulated non-contact atomic force microscopy for polycyclic aromatic hydrocarbons[1] JAMES CHELIKOWSKY, MINJUNG KIM, University of Texas at Austin — Theoretical simulations of non-contact atomic force microscopy (AFM) play an important role in analyzing measured images. Recent non-contact AFM studies on polycyclic aromatic hydrocarbons have achieved atomic resolution that is not observed in other imaging techniques such as scanning tunneling microscopy. In particular, AFM images for these hydrocarbons have resolved bond orders of individual carbon-carbon bonds. Here we present simulated AFM images for several polycyclic aromatic hydrocarbons and explain the role of molecular functionalized AFM tips. Our work is based on solving the electronic structure problem using real space pseudopotentials constructed within density functional theory.

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