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**Simulated imaging of intermolecular bonds using high throughput real-space density functional calculations** ALEX LEE, The University of Texas at Austin, MINJUNG KIM, Yale University, JAMES CHELIKOWSKY, The University of Texas at Austin — Recent experimental noncontact atomic force microscopy (AFM) studies on 8-hydroxyquinoline (8-hq) assemblies have imaged distinct lines between molecules that are thought to represent intermolecular bonding. To aid the interpretation of these images, we calculate simulated AFM images of an 8-hq dimer with a CO functionalized tip using a real-space pseudopotential formalism. We examine the effects of Pauli repulsion and tip probe relaxation as explanations for the enhanced resolution that resolves these intermolecular force lines. Our study aims to compute *ab initio* real-space images of intermolecular interactions.

Alex Lee  
The University of Texas at Austin

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