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Tip relaxation in atomic force microscopy imaging simulations to resolve intermolecular bonds[1] ALEX LEE, YUKI SAKAI, JIM CHELIKOWSKY, The University of Texas at Austin — Experimental noncontact atomic force microscopy (AFM) studies have reported distinct lines in regions with no electron density for a variety of systems. The appearance of these lines is unexpected because Pauli repulsion is thought to be the dominant factor in the AFM imaging mechanism. These lines have been proposed to represent intermolecular bonding. Recent theoretical studies have shown that accounting for tip probe relaxation can sharpen images and highlight features that make simulations more comparable to experiment. We will apply a similar tip relaxation scheme to our computational method–which uses an *ab initio* real-space pseudopotential formalism with frozen density embedding theory added–to the study of dibenzo[a,h]thianthrene and an 8-hydroxyquinoline dimer to develop our interpretation of imaged intermolecular bonds.

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