Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

***Ab initio* simulations of subatomic resolution images in noncontact atomic force microscopy**[1] MINJUNG KIM, Yale University, JAMES R. CHELIKOWSKY, The University of Texas at Austin — Direct imaging of polycyclic aromatic molecules with a subatomic resolution has recently been achieved with noncontact atomic force microscopy (nc-AFM). Specifically, nc-AFM employing a CO functionalized tip has provided details of the chemical bond in aromatic molecules, including the discrimination of bond order. However, the underlying physics of such high resolution imaging remains problematic. By employing new, efficient algorithms based on real space pseudopotentials, we calculate the forces between the nc-AFM tip and specimen. We simulate images of planar organic molecules with two different approaches: 1) with a chemically inert tip and 2) with a CO functionalized tip. We find dramatic differences in the resulting images, which are consistent with recent experimental work.

[1]Our work is supported by the DOE under DOE/DE-FG02-06ER46286 and by the Welch Foundation under grant F-1837. Computational resources were provided by NERSC and XSEDE.

Minjung Kim
Yale University

Date submitted: 14 Nov 2014 Electronic form version 1.4