Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First Principles Simulation of STM Image and Spectroscopy YU ZHU, McGill University, HONG GUO TEAM — In this talk, we shall present a framework for simulating STM images and transport spectroscopy based on density functional theory (DFT) carried out within nonequilibrium Green's function approach (NEGF). In our model, the STM tip and the sample are treated together on equal footing within the self-consistent NEGF-DFT formalism, in contrast to the usual practice where electronic structure of the tip and sample are calculated separately. The NEGF-DFT formalism allows one to do STM simulation whether the STM tip is far (weak coupling) or close (strong coupling) to the sample. The main implementation issues of this STM simulation tool will be discussed and several examples will be given.

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Date submitted: 02 Dec 2006 Electronic form version 1.4