Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Two-probe theory of scanning tunneling microscopy of single molecules JOHN BUKER, Simon Fraser University, GEORGE KIRCZENOW, Simon Fraser University — Experiments in scanning tunneling microscopy of single molecules adsorbed on substrates have produced topographic maps showing how electron flow through a molecule depends on the position of the STM tip above the molecule. However, in some experimental situations, very different topographic maps are obtained when a molecule is adsorbed at different locations on the substrate [1]. This suggests that the tip position is not the only important determining factor for electron flow through the molecule: It is possible that electron flow also depends strongly on the details of the coupling between the molecule and the substrate. However, theoretical work on STM imaging to date has focussed primarily on the role of the tip-molecule coupling. In this talk we re-examine scanning tunneling microscopy of molecules, treating the tip-molecule coupling and the molecule-substrate coupling on the same footing. Treating both the tip and substrate as probes coupled to the molecule, we find that the STM image of a molecule can be sensitive to the geometry of the molecule-substrate coupling. We obtain distinct topographic maps for various configurations of the stationary probe with respect to the molecule, and explain their differences in terms of the molecular orbitals that mediate electron flow in each case. Work supported by NSERC and the Canadian Institute for Advanced Research.

[1]X.H. Qiu, G.V. Nazin, and W. Ho, Science **299**, 542 (2003).

John Buker
Simon Fraser University

Date submitted: 27 Nov 2004 Electronic form version 1.4