

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Scanning Tunneling Spectroscopy of Molecular Electronics Switches J.W. GADZUK, NIST — Theoretical aspects of STS pertinent to molecular electronics systems are considered. The role of multiple-state scattering resonances localized at variable distances along a one-dimensional wire (part of a parallel array lined upright to form a finite-thickness monolayer adsorbed on a metal electrode) is examined. This provides a plausible model for a mobile ligand or attachment responsible for switching and/or negative differential conductance in a MoIE device. It equates to the formal problem of a discrete state (with internal structure) coupled to a 1-D discretized continuum (of molecular orbital/band states). When the continuum level spacing, an inverse function of the wire length, becomes comparable with other characteristic energies of the system such as the coupling strength, vibrational energies, or resonance width, then the position-dependent spectroscopic signature of the switch will be qualitatively different from the usual Fano resonance profile, in a fashion similar to STM line shapes of Kondo impurities in quantum corrals. This dependence provides a useful systematic quantitative tool helpful in the characterization of the electronic conduction properties of MoIE constructs.

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Date submitted: 01 Dec 2004

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