

Abstract Submitted  
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**Electronic and Vibronic Spectroscopy of Molecular Junctions**

JAMES KUSHMERICK, National Institute of Standards and Technology — Transition voltage spectroscopy and inelastic electron tunneling spectroscopy are used to explore charge transport in molecular junctions. Our recent work has shown that a mechanistic transition occurs from direct tunneling to field emission in molecular junctions. The magnitude of the voltage required to enact this transition is molecule-specific, and thus constitutes a form of spectroscopy. We demonstrate that the transition voltage of a conjugated molecule depends directly on the manner in which the conjugation path is extended. Furthermore using inelastic electron tunneling spectroscopy to measure the vibronic structure of non-equilibrium molecular transport, aided by a quantitative interpretation scheme based on non-equilibrium Greens function/density functional theory methods, we are able to characterize the actual pathways that the electrons traverse when moving through a molecule in a molecular transport junction.

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