Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

On the zero-bias anomaly in K-doped C_{60} on Ag(100) NOAH BRAY-ALI, AMY KHOO, Department of Physics, UC Berkeley, JEFFREY NEATON, STEVEN LOUIE, Department of Physics, UC Berkeley and the Molecular Foundry, Lawrence Berkeley National Laboratory, RYAN YAMACHIKA, ANDRE WACHOWIAK, MICHAEL CROMMIE, JOEL MOORE, Department of Physics, UC Berkeley and the Materials Science Division, Lawrence Berkeley National Laboratory — The fullerene molecule C_{60} is known to undergo a strong Jahn-Teller distortion when electrons are added. Recent STM/STS experiments indicate that a single C_{60} molecule on a Ag(100) surface can be controllably doped with charge-donating potassium atoms; [1] moreover, the experiments suggest that the molecular electronic structure can be tuned so that a single electronic orbital lies near the Fermi level. Starting from a Hamiltonian with parameters inferred from companion density functional theory (DFT) calculations of K_xC_{60} on Ag(100), we use Wilson's numerical renormalization group to compute the spectrum near the Fermi level of a doped C_{60} molecule coupled to a metallic continuum. The result compares favorably with spectroscopic measurements of the zero-bias anomaly and, together with the DFT calculations, explains the electronic structure of this system over a range of dopings.

[1] R. Yamachika, M. Grobis, A. Wachowiak, and M.F. Crommie, *Science* **304**, 281-284 (2004).

Noah Bray-Ali
Department of Physics, UC Berkeley

Date submitted: 06 Jan 2006 Electronic form version 1.4