

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Physical manifestation of the Kohn-Sham energy gap in tunneling currents XIAOGUANG ZHANG, Oak Ridge National Laboratory, ZHONG-YI LU, Institute of Theoretical Physics, Chinese Academy of Science, SOKRATES S. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Density-functional theory in the Kohn-Sham (KS) approximation yields accurate ground-state properties of molecules and solids. The KS energy gap, however, is much smaller than the gap obtained from experiments that entail electronic excitations. Here we point out that the zero-bias differential resistance of metal-insulator-metal structures is a ground state property and demonstrate that the KS gap, which is a feature of the ground-state KS Hamiltonian, acts as the effective tunnel barrier. The theory is validated by three sets of available data for the resistance of SiO₂ films as a function of film thickness.

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Date submitted: 29 Nov 2005

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