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Near-Perfect Conduction through a Single Molecular Orbital in a Ferrocene-Based Molecular Wire MICHAEL S. FUHRER, STEPHANIE A. GETTY , CHAIWAT ENGTRAKUL, LIXIN WANG, LAWRENCE R. SITA, University of Maryland, RUI LIU, SAN-HUANG KE, HAROLD U. BARANGER, WEITAO YANG, Duke University — We have studied the electron transport through metal-molecule-metal junctions formed by electromigration of a gold wire in the presence of two phenylethynyl-based dithiol molecules: one containing a central ferrocene moiety (Fc-OPE), and the other a similar-length phenylethynyl analog (OPE). We find that the bias-dependent differential conductance of Fc-OPE shows Lorentzian peaks at small (less than 100 mV) positive and negative bias, with magnitude exceeding 70% of the conductance quantum G_0. The results demonstrate the expected resonant conduction through an extended orbital network long-predicted (but not previously observed) for a conjugated organic system. In contrast, experiments on OPE show much lower conductance, and a gapped region of several hundred millivolts, consistent with previous experimental results on similar all-organic molecular wires. Density functional theory (DFT) and Green function techniques confirm the existence of a low-lying molecular orbital with high transmission in Fc-OPE. Calculations also predict high conductance in OPE, reproducing the long-standing disagreement between experiment and DFT for all-organic molecular wires. While the results do not resolve this dilemma, they place important constraints on future theoretical explanations.

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