Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Negative Differential Resistance in Covalently-Bridged Carbon Nanotube Junctions K.H. KHOO, Dept of Physics UC Berkeley, Mat Sci Div LBNL, Y.-W. SON, Korea Institute for Advanced Study, Dept of Physics UC Berkeley, Mat Sci Div LBNL, MARVIN L. COHEN, Dept of Physics UC Berkeley, Mat Sci Div LBNL, J.B. NEATON, The Molecular Foundry LBNL, STEVEN G. LOUIE, Dept of Physics UC Berkeley, The Molecular Foundry LBNL, Mat Sci Div LBNL — Recently, negative differential resistance (NDR) was observed in IV characteristics of carbon atomic wires connected across multi-wall carbon nanotubes.[1] Motivated by these results, we calculated IV characteristics of carbon atomic wires covalently bridging capped single-wall armchair carbon nanotubes using an *ab-initio* scattering-state formalism based on density functional theory.[2] Our calculations for carbon chains with an odd number of atoms yield currents orders of magnitude larger than that of even chains, demonstrating clear even-odd behavior. We also observe NDR for odd chains and shorter even chains, in agreement with experiment. The current drop at higher voltages is attributed to an energy mismatch between localized nanotube "cap states" on different leads, possibly a generic feature of carbon nanotube molecular junctions. [1] T. Yuzvinsky *et al., Nano Lett.* 10.1021/nl061671j (2006). [2] H.J. Choi, M.L. Cohen and S.G. Louie, to be published. This work supported by NSF Grant No DMR04-39768 and DOE Contract No DE-AC02-05CH11231. Computational resources from NERSC and SDSC.

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Date submitted: 20 Nov 2006 Electronic form version 1.4