

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Graphene Nanogap for Gate Tunable Quantum Coherent Single Molecule Electronics TOMAS LOFWANDER, ANDERS BERGVALL, KRISTIAN BERLAND, PER HYLDGAARD, SERGEY KUBATKIN, Dep. of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-412 96 Goteborg, Sweden — We present atomistic calculations¹ of quantum coherent electron transport through fulleropyrrolidine terminated molecules bridging a graphene nanogap. We predict that three difficult problems in molecular electronics with single molecules may be solved by utilizing graphene contacts: (1) a back gate modulating the Fermi level in the graphene leads facilitate control of the device conductance in a transistor effect with high on/off current ratio; (2) the size mismatch between leads and molecule is avoided, in contrast to the traditional metal contacts; (3) as a consequence, distinct features in charge flow patterns throughout the device are directly detectable by scanning techniques. We show that moderate graphene edge disorder is unimportant for the transistor function.

¹ A. Bergvall, K. Berland, P. Hyldgaard, S. Kubatkin, and T. Lofwander, Phys. Rev. B. **84**, 155451 (2011).

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Date submitted: 28 Nov 2011

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