Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A QM/MM method for simulating the sequencing of DNA using graphene nanopores: solvent efects on nucleobase selectivity ALEXANDRE ROCHA, GUSTAVO FELICIANO, Universidade Federal do ABC - Brazil, YUHUI HE, Osaka University - Japan, RALPH SCHEICHER, Department of Physics and Astronomy, Uppsala University - Sweden, MAURICIO COUTINHO, Universidade Federal do ABC - Brazil — The possibility of using graphene nanopores for DNA sequencing is driving a significant research effort with the aim of obtaining cheaper, more efficient, sequencing techniques. In this work we will present electronic transport calculations of graphene nanopores used for sequencing DNA strands. We consider both single layer and double layer graphene with different types of functionalization of the pore edges. The simulations were performed using a QM/MM method which allows us to treat the graphene sheet containing the nanopore and a segment of DNA within the pore via ab initio DFT methods (QM) whereas the effects of the water molecules, the counter-ions and the remainder of the DNA strand is taken into consideration using a classical potential (MM). The electronic transport properties along graphene are subsequently calculated using non-equilibrium Green's functions including the classical potential. Different time steps of classical molecular dynamics simulations of the DNA strand passing through the nanopore are considered in order to simulate the translocation process. This way we are able to address the effects of the solvent on the selectivity of the device to different nucleobases using atomistic methods.

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Date submitted: 09 Dec 2011 Electronic form version 1.4