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Simulating DNA sequencing using graphene nanopores: a QM/MM Nonequilibrium Green's function approach ALEXANDRE ROCHA, Institute for Theoretical Physics, Universidade Estadual Paulista (UNESP), Sao Paulo, Brazil, GUSTAVO TROIANO, MAURÍCIO COUTINHO-NETO, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo Andre, Brazil, RALPH SCHEICHER, Uppsala University, Uppsala, Sweden — Graphene is both the thinnest possible membrane and presents exceptional electronic transport properties. This combination could pave the way for applications in devices where high selectivity single molecule detection is required, for example for sequencing DNA. In this work we will present theoretical electronic transport calculations of a possible DNA sequencing device based on graphene nanopores. We consider both single and double layer graphene. 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 density functional theory (QM) whereas the effects of the water molecules, the counter-ions and the remainder of the DNA strand are taken into consideration using a classical potential (MM), in such a way that thousands of atoms can be taken into consideration. The arrangement is allowed to evolve in order to sample the configuration space of different basis, and the electronic transport properties along graphene - from a sample of the frames - are subsequently calculated using non-equilibrium Green's functions taking into consideration the solvent effects in the simulation. The effects of the solvent, counter ions and of different stacked basis will be discussed.

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