Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Model results for graphene electrodes in molecular junctions
CARLO MOTTA, Dept. Materials Science, Università di Milano-Bicocca (Italy), MARIO ITALO TRIONI, CNR – National Research Council of Italy, ISTM (Italy), GIAN PAOLO BRIVIO, ETSF, Dept. Materials Science, Università di Milano-Bicocca (Italy), KIZHAKEYIL LUKOSE SEBASTIAN, IPC Department Indian Institute of Science, Bangalore (India), DANIEL SÁNCHEZ PORTAL, Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center (DIPC) — Graphene is a material with a high potential for nanoelectronic applications as transparent conductive electrode. In view of a graphene-based electronics, a possible way to bridge graphene electrodes is by molecular linkers either organic molecules or graphene-derived systems such as graphene nanoribbons (GNR). In the present work, we investigated the electronic and conductive properties of such junctions for two different devices. First we modeled a photochromic switch based on diarylethene molecules, which can be activated/deactivated by light. We found a large on/off current ratio, which can be improved by modifying the functional groups of the molecule. We then investigated the properties of graphene/GNR/graphene junctions, showing that their conductive properties can be tailored by changing the length and width of the GNR. The calculations have been carried out by using the non-equilibrium Green's function method combined with density functional theory.

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Date submitted: 22 Dec 2011 Electronic form version 1.4