Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Room temperature stable single molecule rectifiers with graphite electrodes IVAN RUNGGER, National Physical Laboratory, Teddington, TW11 0LW, UK, V. KALIGINEDI, University of Bern, Switzerland, A. DROGHETTI, Universidad del Pais Vasco, Spain, H. OZAWA, Chuo University, Japan, A. KUZUME, University of Bern, Switzerland, M. HAGA, Chuo University, Japan, P. BROEKMANN, A. V. RUDNEV, University of Bern, Switzerland — In this combined theoretical and experimental study we present new molecular electronics device characteristics of unprecedented stability at room temperature by using electrodes based on highly oriented pyrolytic graphite with covalently attached molecules. To this aim, we explore the effect of the anchoring group chemistry on the charge transport properties of graphite/molecule contacts by means of the scanning tunneling microscopy break-junction technique and ab initio simulations. The theoretical approach to evaluate the conductance is based on density functional theory calculations combined with the non-equilibrium Greens function technique, as implemented in the Smeagol electron transport code [1]. We also demonstrate a strong bias dependence and rectification of the single molecule conductance induced by the anchoring chemistry in combination with the very low density of states of graphite around the Fermi energy. We show that the direction of tunneling current rectification can be tuned by anchoring group chemistry.

[1]A. Rocha et al., Nature Mater. **4**, 335 (2005); A. Rocha et al., Phys. Rev. B **73**, 085414 (2006); I. Rungger et al., Phys. Rev. B **78**, 035407 (2008)

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Date submitted: 12 Dec 2016 Electronic form version 1.4