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Electronic transport through single molecules: effects of strain and contacts HELIO CHACHAM, RONALDO BATISTA, MARIO MAZZONI, Departamento de Fisica, ICEx, Universidade Federal de Minas Gerais, Brazil, IGNACIO GARZON, Instituto de Fisica, Universidad Nacional Autonoma, MARCELA BELTRAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, PABLO ORDEJON, Intitut de Ciencia de Materials de Barcelona, EMILIO ARTACHO, Department of Earth Sciences, University of Cambridge — We will present theoretical investigations on single-molecule electron transport. We will focus on the following systems: a) Connected Au nanoparticles: we performed a first principles study [1] of the electronic properties of lattices of Au nanoparticles functionalized by the conjugated molecules BDMT and BDCT. Distinct behaviors of the electron hopping matrix elements between particles as a function of compression are predicted for functionalized lattices. b) Current rectification with symmetric molecules: In an interesting experiment, Reichet et al. [2] measured the current through symmetric organic molecules and obtained asymmetric IV curves when the Au contacts are pulled apart. We show, by means of first-principles calculations, that this effect can originate from the formation of small Au chains between the molecule and the Au surfaces in an asymmetric way. [1] R. J. C. Batista et al, Phys. Rev. Lett. 96, 116802 (2006). [2] J. Reichet et al., Phys. Rev. Lett. 88, 176804 (2002).

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