Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Fast electron transfer at molecule-substrate interfaces GUIDO FRATESI, ETSF, CNISM, Materials Science Dep., Univ. Milano-Bicocca, Milano, Italy, CARLO MOTTA, School of Physics and CRANN, Trinity College, Dublin 2, Ireland, MARIO ITALO TRIONI, CNR - National Research Council of Italy, ISTM, Milano, Italy, DANIEL SANCHEZ-PORTAL, Centro de Física de Materiales CSIC-UPV/EHU, Donostia-San Sebastian, Spain, GIAN PAOLO BRIVIO, ETSF, CNISM, Materials Science Dep., Univ. Milano-Bicocca, Milano, Italy — The development of efficient organic electronic devices depends substantially on the electronic coupling of the molecules at interfaces and on their arrangement at the nanometer length-scale. As an example, π-conjugated electronic systems maximize their coupling to a contact when they adsorb flat. An effective molecule-substrate interaction is mandatory for solar cells where excited electrons should be collected before recombination. Core electron spectroscopies are possibly the most suitable experimental technique to access fast electron transfer times, but introduce significant perturbation on the valence orbitals by the presence of core holes and bound excitons, further calling for theoretical analysis. This talk will focus on the investigation of elastic electron transfer processes at the molecule-substrate interface based on first-principles Green's function methods. For the electronic coupling of chromophores at semiconductor interfaces we concentrate on the linewidth for electrons excited in molecular LUMO states, as occur in photovoltaic devices or in resonant core spectroscopies, and discuss the effect of core-level excited atoms on the system properties.

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Date submitted: 15 Nov 2013 Electronic form version 1.4