Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Computational investigation of electrode effects in molecular electronics MANUEL SMEU, Binghamton University — The field of molecular electronics offers an avenue to reach the next generation of electronic devices due to the high tunability and relatively inexpensive manufacturing costs of molecules. The field has advanced to the point where molecular junctions can be routinely fabricated and their conductance measured. In terms of computational studies, the state-of-the-art is the non-equilibrium Green's function technique combined with density functional theory (NEGF-DFT) approach that provides the transmission function, $T(E)$, from which the conductance characteristics of the molecular junction can be obtained. A typical system involves a molecule with some anchoring groups (e.g. thiol, amine) connected to Au electrodes. However, using a different metal (Cu, Pt, Al) for the electrodes results in a different alignment between the molecular orbitals and the Fermi level of the electrodes, thus yielding different transport properties. Additionally, the exact atomic configuration at the electrode/molecule interface can play a dramatic role. In this presentation, the effects on molecular conductance of different metal electrodes, their atomic orientation and configuration will be discussed, and some insights into how to obtain control over these parameters will be offered.

Manuel Smeu
Binghamton University

Date submitted: 11 Nov 2016 Electronic form version 1.4