Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Mechanism of H_2O Induced Conductance Changes in $AuCl_4$ Functionalized CNTs ALTYNBEK MURAT, PSE Division, KAUST, Saudi Arabia, IVAN RUNGGER, STEFANO SANVITO, School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland, UDO SCHWINGENSCHLÖGL, PSE Division, KAUST, Saudi Arabia — Functionalized carbon nanotubes (CNTs) are promising candidates for nanoscale sensors due to their high surface-to-volume ratio and the fact that their properties are very sensitive to perturbations. We employ *ab-initio* self-interaction corrected density functional theory combined with the non-equilibrium Green's function method to study the electronic and quantum transport properties of CNTs functionalized with $AuCl_4$ molecules. In particular, we investigate the electronic structure and characterize the conductance for different concentrations and configurations of randomly distributed $AuCl_4$ with and without the adsorption of H_2O molecules, and propose a mechanism that explains the origin of the recently observed resistivity changes of $AuCl_4$ functionalized CNTs upon H_2O adsorption. We find that the adsorption of H_2O shifts the highest occupied Cl and Au states down in energy and thereby reduces the scattering of the electrons around the Fermi level, hence enhancing the conductivity. Our results help facilitate the development of highly sensitive nanoscale H_2O vapor sensors based on $AuCl_4$ functionalized CNTs.

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Date submitted: 13 Nov 2014 Electronic form version 1.4