Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Determining level alignment and coupling strength in single-molecule junctions with chemically-enhanced Raman spectroscopy[1]
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— Raman spectroscopy can be used at the nanoscale to probe binding geometries [1], molecule concentrations [2], carrier densities [3], and charging effects [4]. In this talk, we use finite-difference total-energy and self-energy corrected density functional theory calculations in conjunction with Landauer framework, to study the Raman spectra and transport properties of model nanoscale interfaces, single-molecule junctions – individual molecules contacted with macroscopic metallic electrodes. In the cases of 4,4' bipyridine/Gold and polyphenylene venylene/Gold junctions, we will show how conductance and chemically-enhanced Raman measurement can be used in conjunction to determine the energy scales controlling electron transport i.e. frontier orbital energies and coupling strength.

[1] Zayak et al, Phys. Rev. Lett. 106, 083003 (2011)
[2] Zayak et al., J. Phys. Chem Lett. 3 (10), 1357-1362 (2012)
[3] Das et al. Nanotechnology , 3, 210 215 (2008)
[4] Li et al., PNAS, 111 (4) 1282-1287 (2014)

[1]The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory (Argonne). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. The U.S. Governme

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Date submitted: 14 Nov 2014 Electronic form version 1.4