Abstract Submitted
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First-Principles Studies of Charge Dynamics in Single-Molecule Junctions at Finite Bias[1] PIERRE DARANCET, Molecular Foundry, LBNL, HYOUNG JOON CHOI, Physics, Yonsei University, JONATHAN R. WIDAWSKY, SCOTT BERKLEY, LATHA VENKATARAMAN, Columbia University, JEFFREY B. NEATON, Molecular Foundry, LBNL — Extending well-established measurements of low-bias conductance of single molecule junctions, new experiments report IV characteristics of organic molecules for biases as high as 1V [1]. Such measurements provide a unique probe of electronic properties of well-defined metal-organic nanointerfaces when driven out-of-equilibrium, and an opportunity to examine a still-missing quantitative theory of out-of-equilibrium charge dynamics at the nanoscale. Here we will present first-principles transport calculations for several amine-Au and pyridine-Au linked junctions at different levels of approximation: first mean-field, and then including electron-electron correlations at equilibrium and out-of-equilibrium. We show that incorporating electronic correlations at equilibrium already leads to a very good agreement with experiments [1], and discuss how these corrections might change out of equilibrium.

[1] Widawsky et al., Nanotechnology (2009).

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