MAR12-2011-000683
Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Electron correlation effects on the diode properties and the local heating

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Single molecular bridge junctions and atomic wires provide one of the best test fields for non-equilibrium transport theories whose progress gives benefits over wide range of physics. Experimental progresses in inelastic tunneling spectroscopy (IETS) and break junction techniques have played very important roles to make this possible. Inelastic scatterings between electrons and phonons give "local heating" of the junctions. The effective temperature due to the local heating was discussed successfully in terms of a fully self-consistent theory treating energy dissipation processes as well as inelastic heat generation on equal footing [1]. Recently, we found two cases where electron correlation gives distinct changes. The first case was found in the local heating problem in the resonant systems, where phonon damping due to its coupling with electron-hole excitation is suppressed by the correlation. The suppression enhances heat release to electrodes leading to the effective temperature suppression [2]. Another example is the single molecular rectifier. First principle NEGF-GGA calculation fails to explain the large rectification ratio (RR) at high bias voltage. Separate GW calculation based on Keldysh Green's function gives clear enhancement of RR over the mean field NEGF results suggesting that RR could be enhanced by the electron correlation effect [3]. Thus latest non-equilibrium transport theories enable us to treat the important physical processes accompanying electric conduction allowing us to make more direct comparisons with experimental phenomena at nano-scale.

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[2] Y. Asai, Phys. Rev. B84, 085436 (2011).
[3] Y. Asai, H. Nakamura, J. Hihath, C. Bruot, and N.J Tao, Phys. Rev. B 84, 115436 (2011).