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Incorporating Exchange-Correlation Effects in Quantum Transport through Nano-scale Junctions

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State-of-the-art computational methods for modelling electron transport in nano-scale junctions are based on effective single-particle approximations such as the Kohn-Sham theory of density functional theory. This methodology has been successfully applied to junctions with strong coupling to the metallic electrodes, but has proved insufficient for less homogeneous junctions where the distinction between the nano-device and the electrodes is more pronounced. In order to obtain a more accurate and rigorous description of exchange-correlation effects in weakly correlated molecular junctions, we have implemented the many-body GW approximation within a transport framework suitable to treat non-periodic systems consisting of an interacting region coupled to infinite non-interacting leads with different chemical potentials. Fundamental trends in the properties of metal-molecule-metal junctions are identified on the basis of simple model calculations. These include renormalization of molecular QP levels due to dynamical polarization effects both in- and out of equilibrium as well as the reduction of QP life-times due to enhanced QP scattering under finite bias conditions. As will be shown, these genuine many-body effects can have a large influence on the junction IV characteristics even for weakly correlated systems. The importance of using a fully self-consistent GW self-energy for quantum transport calculations will be demonstrated. Finally (preliminary) results for more realistic molecular junctions will be discussed. References: K. S. Thygesen and A. Rubio, PRB 77, 115333 (2008); K. S. Thygesen, PRL 100, 166804 (2008); K. S. Thygesen and A. Rubio, arXiv:0810.5214.