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Comparative Study of Quantum Monte Carlo and GW methods of treating electronic correlations in nanoscale junctions CATALIN D. SPATARU, XIN WANG, Columbia University, MARK S. HYBERTSEN, Brookhaven National Laboratory, ANDREW J. MILLIS, Columbia University — We analyze the impact of electronic correlation in nanoscale junctions, focusing on the on-molecule interactions. To discuss the essential physics, we restrict attention to a single resonance coupled to metallic leads and including the local Coulomb interaction, the single-impurity Anderson model. Self-consistent GW results for the linear response conductance, orbital filling and spectral function are compared to numerically exact Quantum Monte Carlo calculations. Our analysis suggests that while the GW approximation may be useful for molecular conductors in the non-resonant tunneling regime, it is not accurate for nanoscale junctions in intermediate to strongly correlated and Kondo regimes.

Catalin D. Spataru
Columbia University

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