

Dynamical correction to Kohn-Sham conductances from static density functional theory

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The discontinuity of the exchange-correlation (xc) potential of density functional theory plays a crucial role in determining the equilibrium density of weakly coupled molecular junctions in the

Coulomb blockade regime. In this regime, however, the conductance of the Kohn-Sham (KS) system can be orders of magnitude larger than the true conductance. Here we demonstrate that

this is due to the lack of dynamical xc effects and show how to correct the KS conductance to obtain the physical conductance. Remarkably, the only quantity needed is the derivative of the static xc potential in the molecular junction. Thus the role of the discontinuity is twofold: to yield

an accurate KS conductance and then to correct it. We provide a coherent picture of Coulomb blockade within DFT without breaking the spin symmetry. By application to two different molecular junctions we further show that the dynamical xc correction always reduces the KS conductance, thus contributing to close the gap between theoretical predictions and experimental measurements.

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