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New density functional for molecular conductance

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The "ab initio" descriptions of molecular conductance are routinely performed using density functionals that have spurious self-interaction. This may cause qualitative and severe quantitative errors in the conductance estimation. In an attempt to rectify the situation, we develop a new exact representation of the exchange-correlation energy, from which a new density functional theory is derived. The new functional has correct long-range behavior combined with a good description of the chemical bond. We show that this new functional excellently describes the polarizability of elongated molecules and yields quantitative electron affinity energies. We further show it has a more physical approach to describe the charge distribution in biased systems. The new method is encapsulated the required derivative discontinuities associated with charge transfer. The implication for a realistic description of molecular conductance is discussed.