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Is Density Functional Theory adequate for quantum transport?[1]

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Density functional calculations for the electronic conductance of single molecules attached to leads are now common. I'll examine the methodology from a rigorous point of view, discussing where it can be expected to work, and where it should fail. When molecules are weakly coupled to leads, local and gradient-corrected approximations fail, as the Kohn-Sham levels are misaligned. In the weak bias regime, XC corrections to the current are missed by the standard methodology. Finally, I will compare and contrast several new methodologies that go beyond the present standard approach of applying the Landauer formula to ground-state DFT.

Self-interaction errors in density functional calculations of electronictransport, C. Toher, A. Filippetti, S. Sanvito, and K. Burke, Phys. Rev. Lett. **95**, 146402 (2005)
The Dramatic Role of the Exchange-Correlation Potential in ab initio Electron Transport Calculations, S-H. Ke, H.U. Baranger, and W. Yang, cond-mat/0609367.
Zero-bias molecular electronics: Exchange-correlation corrections to Landauer's formula, M. Koentopp, K. Burke, and F. Evers, Phys. Rev. B Rapid Comm., **73**, 121403 (2006).
Density Functional Theory of the Electrical Conductivity of Molecular Devices, K. Burke, Roberto Car, and Ralph Gebauer, Phys. Rev. Lett. **94**, 146803 (2005).
Density functional calculations of nanoscale conductance, Connie Chang, Max Koentopp, Kieron Burke, and Roberto Car, in prep.

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