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DFT-based transport calculations for single molecules: Can Coulomb blockade effects be reproduced by local functionals? MAX KOENTOPP, Rutgers University, Dept of Chemistry, KIERON BURKE, UC Irvine, Dept of Chemistry — In principle, time-dependent current density functional theory (TDCDFT) allows for exact calculations of the electronic transport properties of single molecules. In practice, one is forced to make approximations for the exchange-correlation functional employed, and the computationally less costly ground-state DFT in a local approximation (GGA) is used. This introduces errors that can lead to an overestimation of the calculated current by one to two orders of magnitude. The use of local approximations to the exchange-correlation functional also leads to the inability to reproduce Coulomb blockade effects. We will discuss the origin and scope of these errors. Then, model calculations for molecules where Coulomb blockade effects have been observed experimentally will be presented, and the mechanism for the failure to reproduce Coulomb blockade effects will be explained.

[1] M.Koentopp, K.Burke, F.Evers, PRB Rapid Comm. **73**, 121403(R) (2006)

Max Koentopp
Rutgers University, Dept of Chemistry

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