Abstract Submitted
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Testing the Standard Approach for Density-Functional Transport Calculations[1] JUSTIN SMITH, Department of Physics, University of California, Irvine, ZHENFEI LIU, Molecular Foundry and Materials Sciences Division, Lawrence Berkeley National Laboratory, KIERON BURKE, Department of Chemistry, University of California, Irvine — Conductance across a single molecular junction can be calculated via the Landauer formalism. This is the standard approach for density-functional theory calculations of transport, but it requires extremely accurate Kohn-Sham potentials that can only be achieved under certain conditions using accurate functionals. Recent work has shown an example where the standard approach works remarkably well for a site model [1, 2]. In this work, we test the standard approach for one dimension in real space where we can extract numerically exact potentials using density-matrix renormalization group [3].

[1] J. P. Bergfield, Z.-F. Liu, K. Burke, and C. A. Stafford, "Bethe ansatz approach to the kondo effect within density-functional theory," Phys. Rev. Lett., 108, 066801 (2012).
[2] Z.-F. Liu, J. P. Bergfield, K. Burke, and C. A. Stafford, "Accuracy of density functionals for molecular electronics: the anderson junction," Phys. Rev. B (2012).
[3] E. M. Stoudenmire, L. O. Wagner, S. R. White, and K. Burke, "One-dimensional continuum electronic structure with the density-matrix renormalization group and its implications for density-functional theory," Phys. Rev. Lett., 109, 056402 (2012).

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