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Electron localization in exact time-dependent density-functional potentials MATTHEW HODGSON, JAMES RAMSDEN, University of York, Department of Physics, THOMAS DURRANT, JACOB CHAPMAN, University College London, Department of Physics and Astronomy, PIERS LILLYSTONE, University of Waterloo, Department of Physics and Astronomy, REX GODBY, University of York, Department of Physics — By propagation of the exact many-electron wavefunction, we determine exact Kohn-Sham (KS) potentials for 1D systems with strong correlation [1]. From this we have developed a density functional which incorporates several features, present in the exact KS potential, that are entirely missing from the usual approximations made in time-dependent density-functional theory (TDDFT) [2]. We find a strong and time-dependent self-interaction correction, owing to electron localization, as well as large static and dynamic spatial steps in the KS potential. Our new functional, suited to simulating ground-state and time-dependent electronic systems, combines an expression for the exact KS potential in the limit of complete electron localization with a measure of the actual localization. Self-consistent application of the functional provides accurate densities for a range of systems, even where the KS potential requires non-local dependence on the charge density, such as potential steps; the self-interaction correction is accurately described. We explore the relationship between features in the KS potential and the "derivative discontinuity."

[1] M. J. P. Hodgson *et al.* **Phys. Rev. B** 88, 241102(R)
[2] M. J. P. Hodgson *et al.* **arXiv:1409.5666**

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