

Abstract Submitted
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Polarizabilities and Hyperpolarizabilities of Hydrogen Chains: Is Self-Interaction Correction the Key? A. RUZSINSZKY, J.P. PERDEW, Dept. of Physics, Tulane U., G.I. CSONKA, Dept. of Chemistry, Budapest U. of Technology and Economics, G.E. SCUSERIA, Dept. of Chemistry, Rice U., O.A. VYDROV, Dept. of Chemistry, MIT — Semi-local density functionals like the local spin density and generalized gradient approximations are known to overestimate [1, 2] the polarizabilities and especially the hyperpolarizabilities of long-chain molecules, while these quantities are much better predicted by exact-exchange methods (Hartree-Fock or Optimized Effective Potential). The source of this failure of the semilocal approaches for the electric response is rooted in the self-interaction error inherent to the semilocal approximations. We show here that the semi-local functionals, after full or scaled-down Perdew-Zunger self-interaction correction [3, 4], are even better than the exact-exchange methods for these quantities.

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Adrienn Ruzsinszky
Dept. of Physics, Tulane U.

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