Abstract Submitted
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Constraint-based, Non-empirical Parameterization of Generalized Gradient Approximation Kinetic Energy Functionals[1] DEBAJIT CHAKRABORTY, SAMUEL TRICKEY, VALENTIN KARASIEV, Department of Physics & Quantum Theory Project, Univ. of Florida — Though we have developed constraint-based "modified conjoint" generalized gradient approximation forms for the orbital-free Kohn-Sham kinetic energy $T_s[n]$, strategies for parameterizing them without use of small training sets have remained elusive[1]. Here we discuss one possible way to eliminate that empiricism. We take the reparameterized Perdew-Burke-Ernzerhof exchange functional PBEmol [2], which is self-interaction free for the Hydrogen atom density n_1. We then constrain the Pauli-term kinetic energy (T_θ in $T_s = T_W + T_\theta$, with T_W the von Weizsäcker KE) to cancel the remaining spurious correlation energy $T_\theta[n_1] + E_{c,PBEmol}[n_1] = 0$.We bound the functional by $T_W + T_{TF}$, with T_{TF} the Thomas-Fermi KE and retain the original constraint that $T_\theta > 0$. We report numerical results and findings for this procedure.

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[2] J. Chem. Phys. **136**, 104108 (2012)

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