Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Stringent test for non-additive, non-interacting, kinetic energy functionals KAILI JIANG, JONATHAN NAFZIGER, Department of Physics and Astronomy, Purdue University, ADAM WASSERMAN, Department of Chemistry, Purdue University — Partition Density Functional Theory (PDFT) provides an ideal framework for testing and developing new approximations to the non-additive and non-interacting kinetic energy functional ($T_s^{nadd}[\{n_\alpha\}]$), understood as a functional of the set of fragment ground-state densities. We present our progress on both of these fronts: (1) Systematic comparison of the performance of various existing approximations to $T_s^{nadd}[\{n_\alpha\}]$; and (2) Development of new approximations. We find that a re-parametrization of the GGA enhancement factor employed for the construction of $T_s^{nadd}[\{n_\alpha\}]$ through the conjointness conjecture captures essential features of the functional derivatives of $T_s^{nadd}[\{n_\alpha\}]$. A physically-motivated two-orbital approximation for $T_s^{nadd}[\{n_\alpha\}]$ is shown to outperform most other approximations for the case of He_2, and an intriguing one-parameter formula makes this approximation accurate for all noble-gas diatomics.

Kaili Jiang
Department of Physics and Astronomy, Purdue University

Date submitted: 03 Nov 2015 Electronic form version 1.4