Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

On the transferability of a parametrized kinetic functional for orbital-free density functional theory calculations ALEXANDER KARPENKO, LEONARDO ESPINOSA LEAL, MIGUEL CARO, JOUKO LEHTOMAKI, OLGA LOPEZ-ACEVEDO, Aalto Univ — Because of issues with accuracy and transferability of existing orbital-free (OF) density functionals, OF functional development remains an active research area. Due to numerical difficulties, all-electron self-consistent assessment of OF functionals is limited. Using the projector augmented wave method we compute OFDFT all-electron values [1] and we evaluate the performance of a parametrized OF functional for atoms and molecules. We combine the parametrized Thomas-Fermi-Weizsäcker (TF-W) kinetic model λ and γ for the fractions of Weizsäcker and TF functionals, respectively, with LDA for atoms [2]. We found that one-to-one relation between λ and γ values defines a region in parameter space that allows the atomic energies and eigenvalues to be approximated with a small average error with respect to the Kohn-Sham values. The optimum values is however different for every property and for every atom. Recently, these results have been combined to test parameter transferability from atoms to molecules [3] and we expect will help for further systematic improvement of OF density functionals.

[1]Lehtomaki *et al.*, JCP., 141, 234102 (2014).
[2]Espinosa *et al.*, PCCP., (2015).
[3]Karpenko *et al.*, in preparation.

Alexander Karpenko
Aalto Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4