Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Towards a kinetic energy density functional for the water molecule OMOLOLU AKIN-OJO[1], DOYIN SHITTU, Department of Physics, Univ. of Ibadan — Development of an accurate kinetic energy kinetic energy density functional (KEDF) is a holy grail. In this work, local KEDFS are parameterized for the water molecule in order to reproduce Kohn-Sham density functional theory (KS-DFT) results. Energies, forces and dipole moments from these KEDFs are presented. Problems with the convergence of the self-consistent-field (SCF) calculations are discussed together with possible solutions.

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Date submitted: 11 Nov 2016 Electronic form version 1.4