Investigation of Kinetic Functionals applied to metal nanoparticles

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In this contribution I present a study of Laplacian-level kinetic energy functionals [1] applied to metallic nanosystems [2]. The nanoparticles are modeled using jellium spheres of different sizes, background densities, and number of electrons. The ability of different functionals to reproduce the correct kinetic energy density and potential of various nanoparticles is investigated and analyzed in terms of semilocal descriptors. I find that the Laplacian contribution is fundamental for the description of the energy (and potential) of nanoparticles.

References:

[1] *Laplacian-level kinetic energy approximations based on the fourth-order gradient expansion: Global assessment and application to the subsystem formulation of density functional theory* S. Laricchia, L. A. Constantin, E. Fabiano, F. Della Sala J. Chem. Theory. Comput. 10, 164 (2014)

[2] *Electronic shell structures in bare and protected metal nanoclusters*, Hannu Häkkinen (2016) Advances in Physics: X, 1:3, 467-491

Figures