

Abstract Submitted
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Nonspherical model density matrices for Rung 3.5 exchange-correlation functionals¹ AUSTIN AGUERO², Angelo State University, BENJAMIN JANESKO, Texas Christian University — Kohn-Sham (KS) density functional theory models electrons' complicated many-body interactions using exchange-correlation density functionals. Semilocal functionals, rungs 1-3 on the “Jacob’s Ladder” of approximate exchange-correlation functionals, model the XC energy density at each point r using information from an infinitesimal region about r . Nonlocal fourth-rung exchange functionals incorporate a dependence on the entire one-particle density matrix of the noninteracting KS reference system. Nonlocal functionals provide improved accuracy for many properties, but have higher computational costs, particularly in extended systems. “Rung 3.5” exchange functionals incorporate the product of the KS density matrix with a semilocal model density matrix, balancing the strengths and limitations of semilocal and nonlocal approximations. This work proposes new semilocal model density matrices for Rung 3.5 functionals. Semilocal density matrices containing 1-3 parameters improve upon previous work for both molecular thermochemistry and kinetics, and show promise for development of future non-empirical Rung 3.5 Density Functionals.

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