Abstract Submitted
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Assessment of a New Semilocal Density Functional on Molecules and Solids[1] YUXIANG MO, JIANMIN TAO, Temple Univ — We have recently developed a new semilocal density functional based on the exchange hole (localized under a general coordinate transformation) from density matrix expansion, instead of imposing energy constraints to the functional or fitting it to a training set of properties. This functional is comprehensively evaluated on diverse properties of molecules and solids, including atomization energies for G2/97 (148 molecules), enthalpies of formation for G3-3 (75 molecules), ionization potentials for G3/99 (86 species), electron affinities for G3/99 (58 species), proton affinities (8 molecules), bond lengths for T-96R (96 molecules), vibrational frequencies for T-82F (82 molecules), 10 hydrogen bonded complexes, as well as lattice constants, bulk moduli, and cohesive energies for solids. Our tests show that the functional is remarkably accurate for these wide-ranging properties.

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