Abstract Submitted
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MN15-L and MN-15: New Kohn-Sham Density Functionals with Board Accuracy for Main-Group and Transition Metal Chemistry and Noncovalent Interactions[1] HAOYU YU, Department of Chemistry, University of Minnesota, XIAO HE, East China Normal University, DONALD G. TRUHLAR, University of Minnesota, DONALD G. TRUHLAR TEAM — The accuracy of Kohn-Sham density functional theory depends on the exchange-correlation functional. Local functionals depending on only the density (ρ), density gradient (grad), and possibly kinetic energy density (τ) have been popular because of their low cost and simplicity, but the most successful functionals for chemistry have involved nonlocal Hartree-Fock exchange (hybrid functionals). We have designed a new meta gradient approximation called MN15-L and a new hybrid meta gradient approximation called MN15 and tested them systematically for 17 absolute atomic energies, 51 noncovalent interaction energies, 56 data on transition metal atoms and molecules, and for 298 other atomic and molecular energetic data, including main-group and transition metal bond energies, ionization potentials, proton affinities, reaction barrier heights, hydrocarbon thermochemistry, excitation energies, and isomerization energies. When compared with 84 previous density MN15 and MN15-L give respectively the smallest and second smallest mean unsigned errors (MUEs, in kcal/mol) on all 422 data with errors for the 4 subsets above being: MN15: 6, 0.26, 4.4, 1.6; MN15-L: 7, 0.45, 4.3, 2.0. Third best: M06: 4, 0.35, 7.7, 2.2. Best previous local functional: M06-L: 7, 0.42, 6.0, 3.5. Other popular functionals: B3LYP: 18, 0.82, 8.2, 4.3; HSE06: 33, 0.58, 8.8, 3.6; TPSS: 18, 0.89, 7.25, 5.0; PBE, 47, 0.88, 9.1, 6.0. MN15-L also performs well for solid-state cohesive energies.

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Haoyu Yu
Department of Chemistry, University of Minnesota

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