

Abstract Submitted
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Better GGA and meta-GGA Functionals: VT84, meta-VMT, meta-VT84¹ ALBERTO VELA, Cinvestav, Mexico DF Mexico, J. MARTIN DEL CAMPO, J.L. GAZQUEZ, Univ. Autonoma Metropolitana I., Mexico, S.B. TRICKEY, Physics, QTP, Univ. Florida — The goal of fast DFT calculations on large families of highly complicated systems (e.g. large clusters, biomolecules) implicitly conflicts with the heavy emphasis of recent years on inclusion of exact exchange. In response we have worked on improving non-empirical GGA X functionals. Here we report extension of our VMT GGA functional (J. Chem. Phys. **130** 244103 (2009)) to satisfy a relevant asymptotic constraint, yielding the VT{84} X functional. With the PBE C functional, VT{84} gives about 10% improvement over VMT in energetics on the G3 223 molecule set. At the meta-GGA level of complexity, we have both meta-VMT and meta-{84}. The former is about 10% better on the G3 set than the TPSS meta-GGA, while meta-VT{84} gives roughly 10% further improvement over meta-VMT. Details of these assessments, including improvements in chemical shifts, will be presented.

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