Abstract Submitted
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Improved Constraint-based GGA Functionals in Extended Systems and Molecules[1] SAM TRICKEY, QTP and Dept. Physics, Univ. Florida, A. VELA, Quimica, Cinvestav, Mexico City Mexico, JUAN PACHECO KATO, Quimica, Univ. Guanajuato, Mexico — Despite wide-spread interest in explicitly orbitally-dependent exchange-correlation functionals, there is aimed at the basic vision of Density Functional Theory, orbital-free implementation. Here we report on further development of our non-empirical X functionals. We give results for the VMT functional (J. Chem. Phys. **130** 244103 (2009)) combined with the PBE C functional on simple solids and ultra-thin films. We also give results for molecules for a more sophisticated family of functionals, VPTmn, which satisfy more constraints than VMT. VMT11 with PBE C tested on a widely used 20 molecule set shows essentially no change in atomization energies compared to VMT, an illustration that enforcing more constraints does not necessarily improve outcomes. We also consider VMT11 in extended systems and in combination with both the LYP and rev-TCA correlation functionals on molecules.

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