Abstract Submitted
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**Self-consistent Meta-GGA for Solids, with Application to the CO Adsorption Puzzle**[1] JIANWEI SUN, JOHN PERDEW, Physics Department, Tulane University, MARTIJN MARSMAN, GEORG KRESSE, Computational Materials Physics, University of Wien — A new proposed meta-GGA in density functional theory (DFT), the revTPSS,[2] unites the advantages of PBEsol and TPSS, giving good lattice constants, as well as good surface and atomization energies. Perhaps the enthusiasm to implement TPSS self-consistently was hindered by its errors in lattice constants (only slightly smaller than the errors of standard GGA's), which might also cause TPSS not so widely adopted for solid calculations. With the improvement of the lattice constants, revTPSS becomes the potential workhorse for both condensed matter physics and quantum chemistry. We implement the revTPSS self-consistently in the VASP code with application to the CO adsorption puzzle. The preliminary results on the site preference and adsorption energy of CO on metallic surfaces look promising. Some standard benchmarking tests, such as lattice constants, bulk moduli, and atomization energies, will also be presented.

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[2]J.P. Perdew, *et al*, Phys. Rev. Lett. **103**, 026403(2009).

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