Abstract Submitted
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Improved Description of Stereoelectronic Effects Using Semilocal Density Functional Theory GABOR I. CSONKA, Dept. of Chemsitry, Budapest U. of Technology and Economics, Budapest, Hungary, JOHN P. PERDEW, ADRIENN RUZSINSZKY, Dept. of Physics, Tulane U., New Orleans LA 70118 — Proper description of stereoelectronic (SE) effects is desirable for any theoretical method to be used in organic chemistry. The SE design rules are frequently used in synthetic organic chemistry to design and explain new reactions by electron donating and withdrawing effects or steric interactions. These effects are often poorly described by standard generalized gradient approximations for exchange and correlation. Many popular exchange-correlation functionals are biased toward the correct description of free atoms and fail to improve upon LSDA for solids. Changing two parameters within the PBE form to satisfy different constraints leads to a new non-empirical GGA, PBEsol [1], that performs well for solids and improves the description of large organic systems and reactions. We present examples where this new non-empirical functional provides considerable improvements for molecules.
[1] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, and K. Burke, http://arxiv.org/abs/0711.0156

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