New Meta-GGA "Workhorses" in Transition Metal Chemistry and SAPT

Marcin Modrzejewski,[a] Michal Hapka,[b] Grzegorz Chalasinski,[c] and Malgorzata M. Szczesniak[d]

[a] *Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic,* [b] *Department of Chemistry, University of Michigan, Ann Arbor, Michigan, USA,* [c] *Faculty of Chemistry, University of Warsaw, Warsaw, Poland,* [d] *Department of Chemistry, Oakland University, Rochester, Michigan, USA*
bryant@oakland.edu

The recently developed DFT meta-GGAs and their hybrids, such as SCAN, SCAN0, MVS, ωB97M-V, and our own LC-PBETPSS-D3, promise improvement over the well-established GGAs and hybrid GGAs developed some 10-20 years ago. Are these promises fulfilled? Most of the tests thus far have involved main-group chemistry (and from the first two periods). This work examines performance of these new methods in transition-metal chemistry and catalysis. The results are rationalized in terms of fractional charge/fractional spin errors. The issue of suitability of these new meta-GGAs in symmetry-adapted perturbation theory is also explored.

References

M. Modrzejewski, G. Chalasinski, and M. M. Szczesniak, *J. Phys. Chem. C* **123** (2019), 8047.