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

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The recently developed DFT meta-GGAs and their hybrids, such as SCAN, SCAN0, MVS, \(\omega\)B97M-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