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Insensitivity of the error of the minimally empirical hybrid functional revTPSSh to its parameters

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Abstract

We investigate the parameter dependence of the error of the hybrid of the revised Tao-Perdew-Staroverov-Scuseria (revTPSSh) density functional for the exchange-correlation energy within popular molecular test sets. In particular, we allow for satisfaction of a possibly tighter Lieb-Oxford lower bound on the exchange-correlation energy. We are able to improve over the original revTPSSh on average, but in total the variation of the performance of revTPSSh seems to be low when its parameters are changed. We recommend to continue using the original revTPSSh variant rather than our fitted versions, because we expect a broader applicability from the original parameter set. (C) 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4769790>]

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