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Semilocal Density Functional with High Accuracy for Molecules and Solids[1] JIANMIN TAO, Temple University, GUOCAI TIAN, Kunming University of Science and Technology, YUXIANG MO, Temple University — Kohn-Sham density functional theory is the most popular electronic structure theory, due to the excellent balance between computational cost and improvable accuracy. Recently, we have proposed a nonempirical semilocal density functional [1] based on the exchange-correlation hole. The exchange part was essentially derived from the density matrix expansion, while the correlation part is obtained from a modification of the TPSS correlation in the low-density limit. In this talk, I will present our extensive assessment of the performance of this functional on molecules and solids.
[1] J. Tao and Y. Mo, PRL 117, 073001 (2016).

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