An Accurate Density Functional from Exchange-Correlation Hole

JIANMIN TAO, YUXIANG MO, Temple Univ — The exchange-correlation hole is most fundamentally important in the development and understanding of density functional theory (DFT). However, due to the nonlocal nature of the exchange-correlation hole, development of DFT from the underlying hole presents a great challenge, and the works along this direction are limited. Here I will discuss a novel nonempirical DFT based on a semilocal hole, which is obtained from the density matrix expansion. Extensive tests on molecules and solids show that this functional can achieve remarkable accuracy for wide-ranging properties in condensed matter physics and quantum chemistry.

This work was supported by NSF under Grant No. CHE-1261918

Jianmin Tao
Temple Univ

Date submitted: 06 Nov 2015