

Abstract Submitted  
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**An Accurate Density Functional from Exchange-Correlation Hole**<sup>1</sup> 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.

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