

Angular-Momentum Dependent Orbital Free Density Functional Theory

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Orbital-free (OF) density functional theory (DFT) directly solves for the electron density rather than the wave function of many electron systems, greatly simplifying and enabling large scale first principles simulations. However, the required approximate noninteracting kinetic energy density functionals and local electron-ion pseudopotentials severely restrict its general applicability. To solve this problem, we have developed angular-momentum-dependent (AMD)-OFDFT [1], which combines the accuracy of Kohn-Sham DFT with the numerical prowess of OFDFT. The angular momenta of electrons are explicitly introduced within atom-centered spheres so that the important ionic core region can be accurately described. In addition to conventional OF total energy functionals, we introduce a crucial nonlocal energy term with a set of AMD energies to correct errors due to the kinetic energy density functional and the local pseudopotential. We present results for different phases of the transition metal titanium, as well as vacancies and surfaces. We benchmark our results against state-of-the-art Kohn-Sham calculations, and find substantial improvement compared to conventional OFDFT formulations.

[1] Y. Ke, F. Libisch, J. Xia, L.-W. Wang, and E. A. Carter, Phys. Rev. Lett. 111, 066402 (2013)