Development and Applications of Orbital Free Density Functional Theory

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Recent advances from the University of Florida Orbital Free Density Functional group are surveyed. The group's broad objective is accurate, practical, formally sound implementation of density functional theory (DFT) for application to the challenging state conditions of "warm, dense matter". Practical limitations of the conventional Kohn-Sham method at temperatures at or above the Fermi temperature require a return to the original Hohenberg-Kohn-Mermin form in terms of functionals of the density alone. Recently, the UF group has constructed a non-empirical free energy functional from its non-interacting and exchange-correlation (XC) components. Construction exploited established T=0 generalized gradient approximations (GGA), the finite-T gradient expansions (GE) for both non-interacting and XC terms, and exact finite T limits. The result is a new GGA bridging low-T (ground state) and high-T (plasma) limits." Accuracy of the new XC functional in the WDM regime is illustrated by deuterium equation of state calculations in excellent agreement with reference path integral Monte Carlo results at intermediate and elevated T. Accuracy of the non-interacting functional is attested by direct comparison with conventional Kohn-Sham calculations.

All of our functional developments are available in our PROFESS@QuantumEspresso package. Its libraries and code couple PROFESS version 3.0 with QuantumEspresso version 5.2.1. The result enables orbital free DFT (OFDFT) ab initio molecular dynamics (AIMD) simulations in modified QuantumEspresso on the same technical footing (MD algorithms, thermostats, parameters, etc.) as for Kohn-Sham DFT.

Transport, specifically the electron conductivity, has been addressed within the Kubo-Greenwood approximation. The current-current time correlation function is computed for mean-field Kohn-Sham dynamics at sampled time steps for the fully correlated ion dynamics. The time steps are from classical molecular dynamics with OFDFT forces (AIMD). Solutions to both formal and technical problems implicit in the use of Projected Augmented Wave datasets and a plane wave basis have been addressed. Implementation (open-source Fortran 90 code) is as a post-processing tool for QuantumEspresso. Beta testing is underway and illustrative initial results published.

Software and publications are available from www.qtp.ufl.edu/ofdft.

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