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Angular Momentum Dependent Orbital Free Density Functional Theory YOUQI KE, FLORIAN LIBISCH, JUNCHAO XIA, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA, LIN-WANG WANG, Material Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, EMILY A. CARTER, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA — We report a novel and general formalism for linear scaling, angular momentum dependent (AMD) orbital free (OF) density functional theory (DFT) to advance the accuracy and applicability of OFDFT. To introduce angular momentum dependence in OFDFT, we devise a hybrid scheme by partitioning the system into muffin-tin spheres and an interstitial region: the electron density inside the spheres is expressed by a set of Kohn-Sham (KS) DFT derived atom-centered basis functions combined with an on-site density matrix N_R. A general OFDFT total energy functional is introduced with a crucial nonlocal energy term E^{NL} which is neglected in conventional implementations of OFDFT. E^{NL} corrects the errors due to the use of approximate kinetic energy density functionals and local pseudopotentials for ion-electron interactions. We approximate E^{NL} to include AMD contributions inside the spheres: as a first step, a linear dependence on the N_R is considered with a set of AMD energies E^l_R. E^l_R are determined by fitting a small set of bulk properties to KSDFT. We find AMD-OFDFT offers substantial improvements over conventional OFDFT, as we show for various properties of the transition metal Ti and its alloys (Ti_xAl_{1-x}).

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