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Efficient optimal effective potential approach for pe- riodic plane-wave density functional theory[1] FLORIAN LIBISCH, JOHANNES M. DIETERICH, CHEN HUANG, EMILY A. CARTER, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA
— Kohn-Sham (KS) density functional theory (DFT) formulates equations for non-interacting electrons subject to a mean-field KS potential. The exchange and correlation (XC) between electrons are accounted for by density-based XC-functionals. The introduction of orbital-dependent functionals allows for a more accurate treatment of exchange and correlation, a prominent example being the exact treatment of Hartree-Fock exchange. Such a construction, however, is not straightforward in KS DFT, as all Kohn Sham orbitals fulfill the same KS equation. For a given orbital-dependent functional, direct solutions to find the corresponding KS potential are numerically cumbersome or even unstable. By extending and combining previous approaches [Phys. Rev. B 62, 15521 (2000), Phys. Rev. B 84, 165122 (2011)], we introduce a momentum-space based formulation that allows for an efficient treatment of orbital-dependent functionals. We include the full spin degrees of freedom, as well as periodic boundary conditions and k-point sampling. We show that for the spin-free case, our formulation becomes similar to the orbital-shift approach [Phys. Rev. B 68, 035103 (2003)] but numerically better suited for implementation in plane-wave DFT codes. Finally, we discuss practical applications.

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