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Large-scale DFT calculations with the ONETEP program on metallic systems ALVARO RUIZ-SERRANO, CHRIS-KRITON SKYLARIS, University of Southampton — We present a direct energy minimization method based on the Kohn-Sham formulation of Mermin's extension of density functional theory (DFT) to finite electronic temperature for large-scale calculations on metallic systems. Our approach employs norm-conserving pseudopotentials for the core electrons, whereas the valence electrons are accurately described using a set of localized orbitals, optimized in-situ in terms of a high-resolution periodic-sinc (psinc) basis set equivalent to plane-waves. The localization constraint results in predictable sparsity patterns that simplify the algebraic operations with matrices, while the description in terms of psinc functions allows near-minimal matrix sizes. As a consequence, the traditional computational bottleneck due to diagonalization of the Hamiltonian matrix is greatly reduced, allowing calculations on larger systems. Additionally, we take advantage of available parallel eigensolvers to enhance the efficiency of the method. We present a number of validation results on metallic systems of increasing complexity and size, including calculations on nanoparticles of more than a thousand atoms.

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