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Large-scale DFT calculations using multi-site support functions in CONQUEST[1] AYAKO NAKATA, National Institute for Materials Science, DAVID BOWLER, University College London, TSUYOSHI MIYAZAKI, National Institute for Materials Science — CONQUEST is a linear-scaling (O(N)) DFT code developed jointly by UCL and NIMS. CONQUEST achieves O(N) by using the locality of density matrices with the density matrix minimization method. Local orbitals which are called support functions are used to express the density matrices and Kohn-Sham orbitals. Our recent study shows that the code can employ DFT calculations on million-atom systems. We have introduced multi-site support functions [Phys. Chem. Chem. Phys. 17, 31427 (2015)], which are the linear combinations of pseudo-atomic orbitals from a target atom and its neighbor atoms. Multi-site support functions correspond to local molecular orbitals so that the number of required support functions can be the minimal. The linear-combination coefficients are optimized numerically while the initial coefficients are determined by using the localized filter diagonalization method [Phys. Rev. B 80, 205104 (2009)]. The accuracy and computational efficiency of the present method are demonstrated by investigating the atomic and electronic properties of hydrated DNA systems containing several thousand atoms. The test calculations of metallic nanoparticles show the applicability of the method to metallic systems.

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