ID: P1.26

Title: Extending the length scales of many-body simulations with density-functional calculations

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We present a method for estimating the finite-size (FS) effects in many-body electronic structure calculations of extended systems by a modified density functional theory (DFT) calculation. The method reduces the need to repeat expensive many-body simulations for different supercell sizes, and accelerates the convergence to the thermodynamic limit. We construct a unified FS DFT exchange-correlation functional for spin unpolarized and fully spin polarized systems, under the local density approximation. The results are then interpolated to arbitrary spin polarizations. Applications are shown to both non-magnetic and magnetic systems. In addition, we have also parametrized the correlation energy of the electron gas as a function of finite kinetic energy cutoffs, by auxiliary-field quantum Monte Carlo calculations. This may be useful for a correction scheme for many-body simulations using smaller basis sets. (Research is supported by DOE, NSF, and ONR.)