Density fitting Hartree calculations for extended systems with translational periodicity

Matúš Milko,[a] Štefan Varga[a] and Jozef Noga[a,b]

[a]Institute of Inorganic Chemistry,
Slovak Academy of Sciences, SK-84536 Bratislava, Slovakia

[b]Faculty of Natural Sciences,
Comenius University, SK-84215 Bratislava, Slovakia

Density fitting approach to the Coulomb problem for infinite systems with translational periodicity was shown to behave correctly by one of us recently[1]. We show that the formulations in reciprocal and direct space are fully equivalent, leading to a compact and easy-to-evaluate formula. Computational demands scale linearly with the number of unit cells. Moreover, our scheme is independent of the Brillouin zone sampling as all the Coulomb interaction information is contained in the Γ-point of the reciprocal space. All this offers an extremely fast scheme for Hartree calculations in the solid state.
A way of auxiliary basis set construction which allows for a systematic improvement of the accuracy is proposed. Its effectiveness is demonstrated on two model 1D periodic systems, trans-polyacethylene and trans-cyanoborane. We show that accuracy at μE_h level can be achieved with a reasonable size of the auxiliary basis set with computer demands beeing a negligible fraction of conventional Hartree calculation.

[1] Š. Varga, *Phys. Rev. B*, 71, 73103, (2005).