O.14 Coulomb cut-off methods in ABINIT ground-state calculations

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Implementations of Density Functional Theory based on plane-waves are intrinsically linked with periodic boundary conditions, as it is the case of the ABINIT package.[1–3] This method is perfectly suitable when describing 3D periodic crystal, but it can become computationally restrictive when describing low dimensional systems, such as slabs (2D), nanowires (1D) or nanoparticles (0D), due to the long range character of the Coulomb-like terms present in the formalism. The effect of the residual Coulomb interaction is usually avoided by using a sufficiently large simulation box along the non-periodic directions. The GW part of ABINIT already employs Coulomb truncation methods to accelerate the converge with respect to the supercell since the self-energy is rather sensitive to the spurious interaction with the periodic images. It should be noted, however, that the GW implementation is not completely consistent as the Green's function G and the screeneed interaction W are still constructed from Kohn-Sham orbitals obtained without any cutoff in the Coulomb interaction. In this work we transfer the current methods suitable for 2D or 1D systems[4,5], respectively 0D[6] to the ground-state level of ABINIT. We present the current status of this ongoing work.

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