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Equivalence of dipole correction and Coulomb cutoff techniques in supercell calculations LIPING YU, V. RANJAN, NC State U, Raleigh, W. LU, J. BERNHOLC, M. BUONGIORNO NARDELLI, NC State U, Raleigh and ORNL, TN — In ab initio calculations for surfaces or non-periodic systems one often relies on the supercell approximation, where periodic replicas are separated by enough empty space to avoid spurious interactions between successive images. However, a vacuum separation is not sufficient to screen dipolar interactions that appear in asymmetrically charged or polar systems. Two solutions have been proposed in the literature: (i) the dipole correction, and (ii) Coulomb cutoff formalism that eliminates interactions between periodic replicas. We compare these methods under the same conditions in the framework of plane wave DFT calculations. It is found that the two methods produce equivalent results for the total energy, force, charge density and self-consistent potential. In band structure calculations, the results coincide for occupied states but differ for delocalized unoccupied ones in small supercells. This discrepancy can be used as a criterion to identify supercell sizes that are sufficiently large to obtain converged results.

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