Supercell Size Scaling of Formation Energies of Charged Defects

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Abstract

We present DFT calculations of defect formation energies in alumina, a ceramic oxide considered for an archetype for other similar oxides. Combining an existing method for the determination of elemental chemical potentials (as a function of the thermodynamic formation conditions), with a new method for extrapolation to effectively infinite-supercell size (removing finite-size errors in electrostatic and elastic energy), we show how the results can be made relatively insensitive to the principal approximations of DFT. These include choices of XC-functional and pseudopotential and the supercell in which we pattern the (non-primitive) 30-atom hexagonal cell of Al₂O₃, set, using the CASTEP code [2]. For the extrapolation to infinite supercell size we obey the constraint of charge neutrality ensures that the net charge 6. For de-