Electrostatics-based finite-size corrections for point defects in semiconductors

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First-principles point defect calculations usually adopt three-dimensional periodic boundary conditions, which can lead to huge errors in charged defect formation energies in semiconductors up to several electronvolts. The main error sources are artificial electrostatic interactions related to periodic images and uniform background charge. Recently, Freysoldt et al. proposed a scheme to accurately construct the finite-size correction energies \textit{a posteriori}. Their original correction scheme, however, uses a dielectric constant that is suitable for isotropic systems. Furthermore, it adopts a planar-averaged potential for determining the potential offset between the defect-induced and model charge potential, which cannot be readily applied to defects with large atomic relaxation associated with electric-field screening.

To remedy these deficiencies, we extend their scheme by rewriting the formalism in an anisotropic form with a dielectric matrix and by using atomic site local potential as a potential marker. The corrective capability was systematically assessed for 17 defects in 10 materials: defect formation energies in diverse materials are excellently corrected within errors of less than 0.2 eV for small supercells containing around 100 atoms.