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Electrostatic screening in supercell calculations of formation energies of charged-defects[1] YUNING WU, Univ of Florida - Gainesville, SOKRATES PANTELIDES, Vanderbilt University, XIAOGUANG ZHANG, Univ of Florida - Gainesville — Density functional theory calculations of the formation energies of charged defects use a uniform compensating (jellium) background to screen the electrostatic interactions between the supercells. This approximation may cause large errors in complex materials where the screening charge may be different on different sublattices. Here we recognize that charged defects exist in overall neutral systems and develop a more realistic approach to calculate formation energies of charged defects. We use density functional theory and calculate formation energies for vacancies in Si, GaN, and ZnO. We find significant differences from the usual calculations in both the neighboring atom displacements and the formation energies. The common unphysical result that vacancy formation energies become negative when the Fermi energy approaches the conduction-band edge is greatly improved.

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