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Charged defects in the supercell approach

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In electronic structure theory, point defects in crystalline materials are usually modelled in the supercell approach. While the isolated-defect limit (i.e. low concentrations) can be achieved by making the supercell large enough in principle, advanced electronic structure methods are limited to rather small system sizes (i.e. excessively high concentrations) in practice. For these small systems, however, defect-defect interactions may significantly alter the calculated properties. In order to apply any advanced method to point defects, the unavoidable artifacts must be corrected for. For charged defects, the Coulomb interaction between the defect and its periodic images as well as the unavoidable neutralizing background gives rise to a slow convergence of the defect energetics with respect to supercell size. Various correction schemes have been suggested over the years, ranging from Coulomb truncation over Makov-Payne corrections to scaling-law extrapolation. Unfortunately, the schemes often disagree and sometimes even worsen convergence with respect to supercell size. I will review these approaches in the light of an exact, yet tractable treatment of the electrostatics in a polarizable material, and present our new correction scheme derived from this analysis with well-controlled approximations [Phys. Rev. Lett. 102, 016402 (2009)].