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Fully *ab initio* supercell corrections for charged defects
CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, Max-Planck-Institut for Iron Research, Duesseldorf, Germany, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara — Charged point defects govern the carrier densities in semiconductors and are crucial for the performance of electronic devices. However, quantifying the thermodynamical, chemical, and electrical properties of such defects is a challenge to both experiment and theory. In *ab-initio* calculations, the defect is usually modeled in a periodic supercell with a few dozen to a few hundred atoms. Unfortunately, this introduces artificial electrostatic interactions between charged defects. A number of correction schemes such as Makov-Payne corrections, potential alignment, scaling laws, or Coulomb truncation, are available in the literature, but they often fail to remove the supercell dependence completely. The assumptions behind these schemes are sometimes unclear and all schemes lack a stringent theoretical foundation. From a formal analysis within linear-response theory, we propose a new and simple scheme that combines the strengths of Makov-Payne corrections and potential alignment. Our scheme requires no empirical parameters or fitting procedures. Its reliability is demonstrated even in extreme cases.

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