

## Insights into why the DFT band-gap problem does not limit the range of energy levels computed for point defects in semiconductors

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Point defects in semiconductors are largely characterized by their levels, which are defined as the Fermi levels at which the equilibrium charge state of the defect changes. Kohn-Sham density-functional theory (DFT) has successfully predicted defect levels for a wide variety of semiconductors and, surprisingly, these levels are often found to span an energy range significantly larger than the DFT gap. One reason for this result is that the range of levels computed using a finite-sized supercell are not limited by the DFT gap, which is defined as the difference in the energies to add and remove one electron to and from infinite bulk, but rather by the energy difference to add and remove one electron to and from the finite-sized bulk supercell corresponding to the one in which the defect calculations are performed. This supercell size-dependent gap is larger than the DFT gap for the same physical reasons that the measured gap in a degenerately doped semiconductor is larger than the measured gap in an undoped semiconductor, namely Moss-Burstein (band filling) effects arising from the large changes in the electron density ( $\pm 2 \times 10^{20}/\text{cm}^3$  for a 216-atom supercell) that occur when adding and removing one electron from a finite-sized supercell.

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