Contribution ID: **528** Type: **Oral Presentation**

Assessing the Freysoldt, Neugebauer & van de Walle (FNV) and Kumagai–Oba (KO) finite-size corrections for Ce-vacancy complexes in diamond

Tuesday 8 July 2025 16:50 (20 minutes)

Lanthanide-doped diamond couples the ultra wide band gap, high thermal conductivity and radiation hardness of the host with the rich $4f$ electron physics of the dopant, promising solid-state qubits, single-photon emitters and spin-memory elements. Supercell density functional theory treatments of the charged Ce-vacancy complexes that underlie these functionalities suffer from spurious image–image interactions and an ill defined electrostatic zero energy; post processing finite-size corrections are therefore mandatory for quantitative defect thermodynamics.

We benchmark the two principal correction schemes—the reciprocal space potential alignment/monopole method of Freysoldt, Neugebauer & van de Walle (FNV) and the real space multipole expansion of Kumagai &Oba (KO)—for Ce_{V2}, Ce_{V3} and Ce_{V4} in a 216-atom diamond supercell. Uncorrected neutral formation energies agree with literature to within 0.5 eV for Ce_{V2} and Ce_{V3} and confirm Ce_{V3} as the most stable neutral complex. Introducing positive charge exposes limitations of FNV: once the anisotropic Ce $4f$ charge density departs from the isotropic monopole assumed in that formalism, FNV corrections fail to converge. In contrast, KO, which accounts for higher multipoles, remains numerically stable and delivers consistent corrections.

Our results show that KO is indispensable for heavy-atom defects with non-spherical charge distributions, while FNV is reliable only for nearly isotropic cases. This enables accurate assessment of rare-earth dopants in diamond and other wide-gap semiconductors.

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Session Classification: Physics of Condensed Matter and Materials 2

Track Classification: Track A - Physics of Condensed Matter and Materials