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Special Displacement Method for Single-Photon Emitters in Diamond and h-BN

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Single-photon emitters (SPEs) are key components for quantum technologies, particularly in sensing and secure communication. In solids, SPEs often originate from point defects that introduce discrete states within the band gap. Electron–phonon coupling can strongly affect these defect levels by renormalizing their energies, thereby shifting the emitted photon energy. Common theoretical approaches to account for electron–phonon coupling, such as Monte Carlo-based methods, are computationally expensive, requiring hundreds to thousands of supercell configurations. The Special Displacement (SD) method proposed by Zacharias et al. offers reliable accuracy at significantly lower computational cost. While successfully applied to pristine materials, its validity for defect systems remains unclear. In this work, we apply the SD method to evaluate electron–phonon coupling in defect structures. We focus on two important SPE systems: the NV^- center in diamond and the carbon dimer defect in h-BN. After validating the SD method for the NV^- center, we apply it to h-BN and compute defect-level renormalization energies and their temperature variation. Furthermore, we explore strategies to further reduce the computational cost of such calculations. By enabling more accurate predictions of emission energies and their temperature dependence, this framework is a step forward toward efficient and predictive modeling of next-generation single-photon emitters.

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