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Ab Initio Investigation of Erbium Point Defects in 4H-SiC for Quantum Emitters

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Erbium-doped 4H-SiC is a promising platform for integrated quantum photonics because the intra-$4f$ transition of Er^{3+} enables telecom-wavelength emission near 1.55 μm, while the wide-bandgap SiC host offers excellent optical properties and compatibility with established semiconductor fabrication processes. However, photoluminescence measurements alone cannot uniquely identify the atomic configuration responsible for emission, limiting the ability to engineer emitters with tailored optical properties [1]. To address this deficiency, we performed first-principles density-functional theory calculations using ABINIT [2] with the Perdew-Burke-Ernzerhof (PBE) exchange–correlation functional, projector augmented-wave (PAW) pseudopotentials, and a Hubbard U correction applied to the Er $4f$ states [3,4].

Eight candidate erbium defect configurations, including substitutional, interstitial, vacancy-associated, and impurity-paired complexes, were screened in 32-atom supercells and ranked by their neutral formation energies. The four most favorable structures were subsequently relaxed in neutral 128-atom supercells and then vertically screened across charge states from $q = -2$ to $+2$. Charged relaxations were then performed for the stable charge states of the lowest energy configuration, and charge-transition levels were calculated, including the Madelung image-charge correction for a finite supercell [5]. For the same configuration, k-resolved Kohn–Sham eigenvalues and projected densities of states were used to characterize the defect levels, their occupations, and their orbital character.

The calculations reveal that isolated substitutional and interstitial erbium defects are energetically unfavorable and that erbium preferentially forms complexes with impurities and carbon vacancies. The lowest-energy configuration is the hexagonal Si-substitutional defect paired with a carbon-site oxygen impurity, $Er_{Si}(h)$+O_C, with a formation energy of 1.08 eV. This structure is energetically favored over the corresponding nitrogen complex (2.12 eV) and over the h- and k-site carbon-vacancy complexes (3.19 and 4.86 eV). The defect exhibits a partially occupied Er $4f$ manifold consistent with the $4f^{11}$ electronic configuration of Er^{3+}, producing strongly localized in-gap states 2.05–2.13 eV above the valence-band maximum, with approximately 94% of the projected orbital character originating from the defect. Furthermore, formation-energy calculations reveal negative-U behavior, with the neutral charge state never becoming thermodynamically stable within the band gap and a single $(+/-)$ transition level predicted near 2.4 eV above the valence-band maximum. These results suggest that the $Er_{Si}(h)$+O_C impurity complex might be a leading candidate for optically active erbium centers in 4H-SiC for the design of quantum emitters near the standard telecom wavelength of 1.55 μm.

References

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