Ab initio STUDY OF VIBRATIONAL PROPERTIES OF DIVACANCY DEFECTS IN 4H-SiC

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Silicon carbide (SiC) is a wide bandgap material with great potential for high-power and high-frequency electronic devices. Furthermore, certain deep-level semiconductor defects have potential applications as qubits and single photon emitters for quantum technologies (QT). SiC hosts a wide variety of defects with QT-compatible properties. In multi-component semiconductors, such as SiC, these defects can often inhabit several configurations with different characteristics. Therefore, a detailed characterization of different defect configurations and their electro-optical properties is essential.

Our study employed first-principles calculations to study four neutral divacancy configurations (*hh*, *kk*, *hk*, and *kh*) and their vibrational properties in the 4H-SiC polytype. The labels *h* and *k* refer to the distinct hexagonal and pseudo-cubic lattice sites in 4H-SiC, respectively. Using the r^{2}SCAN density functional [1][2], we have determined the zero-phonon line (ZPL) energies and zero-field splitting (ZFS) values, which are in close agreement with experimental data [3]. Furthermore, we calculated the spectral functions of electron-phonon coupling using a novel embedding methodology [4][5]. The calculated luminescence lineshapes provide excellent agreement with the experimental data.

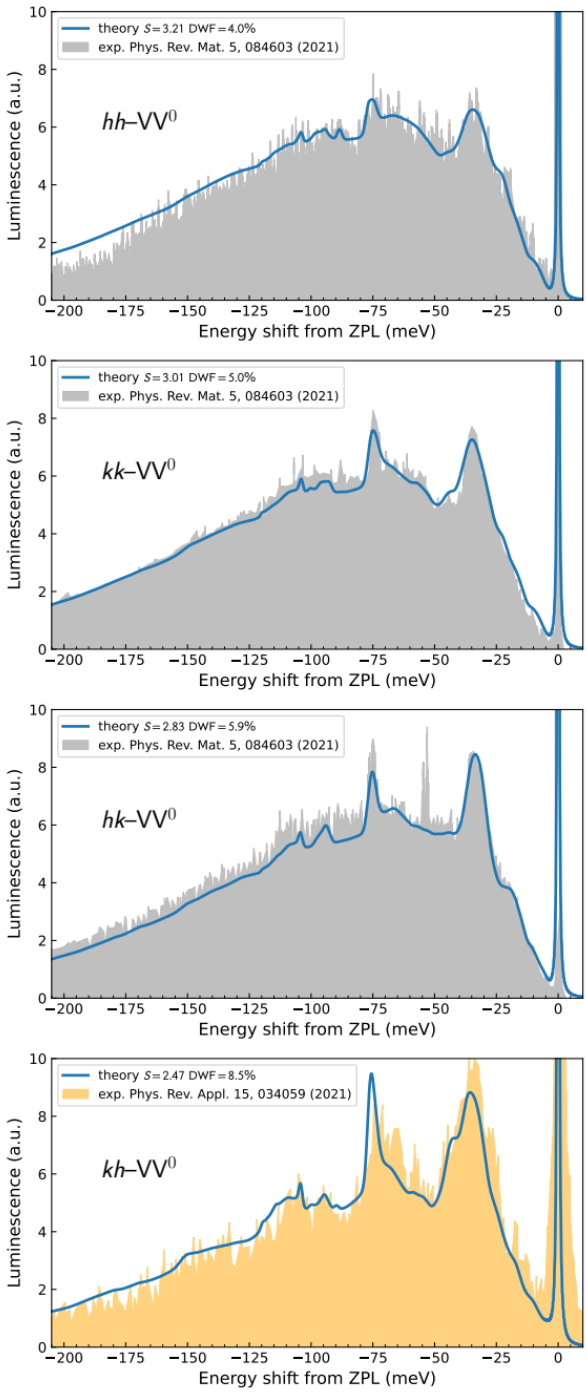

Fig. 1 Calculated theoretical normalized luminescence line shapes of divacancy defects in 4H-SiC compared with experimental data.

References

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