THEORETICAL MODELING OF VIBRATIONALLY RESOLVED OPTICAL LINESHAPES OF A CARBON-OXYGEN PAIR DEFECT IN SILICON

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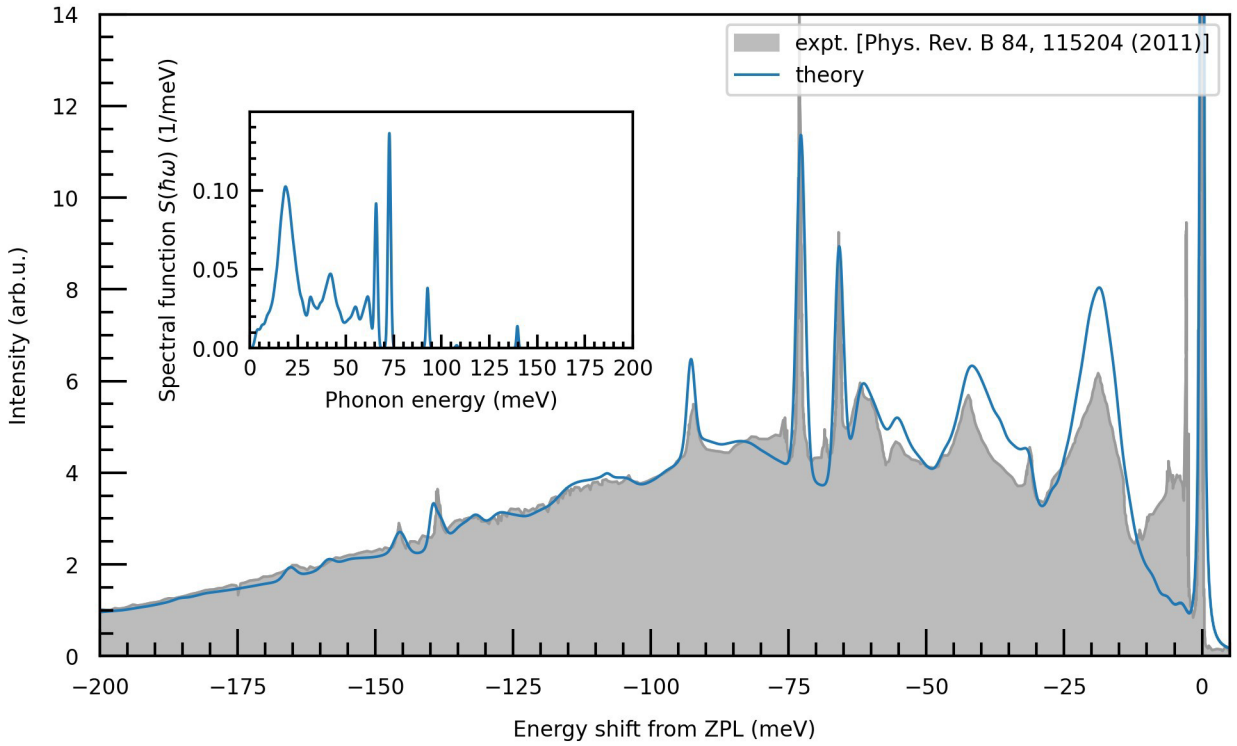

Figure 1. Experimental (gray) and calculated (blue) normalized luminescence lineshapes of C-center in silicon. The inset figure contains the spectral function of electron-phonon coupling.

In recent years, quantum technologies have been at the forefront of scientific interest due to various possible applications in quantum sensing, communication, and computing. Optically active point defects are of particular interest as single-photon emitters that could be used for short- and long-distance exchange of information [1]. The C-center, composed of a carbon-oxygen interstitial pair (CiOi), is one such defect [2, 3, 4]. It emits light at telecom wavelengths of 1570 nm (0.789 eV) and is thus a suitable candidate for a telecom-range single- photon source that is compatible with fiber- optic technology [5].

This work presents a first-principles computational study of the luminescence and absorption lineshapes associated with the C- center in silicon. We perform density functional theory (DFT) calculations with a semilocal functional based on the meta-generalized gradient approximation (meta-GGA) [6], in particular, the recently developed SCAN (Strongly-Constrained and Appropriately- Normed) functional [7]. Using a novel embedding methodology [8, 9], we obtain optical emission (Figure 1) and absorption lineshapes of the defect in the dilute limit. Our results show a close agreement to the experimentally observed luminescence lineshape, while the absorption lineshape data could be used as a guide for further experimental analysis of the C-center.

References

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