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Phonon sideband studies of the spin-triplet optical transition in diamond nitrogen-vacancy centers[1] AUDRIUS ALKAUSKAS, Materials Department, University of California, Santa Barbara, DAVID M. TOYLI, BOB B. BUCKLEY, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — In the past decade, the nitrogen-vacancy center in diamond has emerged as a promising solid-state system for quantum-information processing, and also for nanoscale magnetic, electric, and thermal sensing. All of these applications are partly enabled because the spin of the center can be measured through photoluminescence. This calls for a deeper understanding of the photoluminescence spectrum, in particular its phonon side-band. In this work we study the coupling of lattice vibrations to the triplet ($^3\mathrm{E}\rightarrow{}^3\mathrm{A}_2$) optical transition from first-principles electronic structure calculations. Our formulation includes both quasi-localized and bulk phonons, and leads to an excellent agreement of the calculated and the measured photoluminescence lineshape. This good agreement enables the application of the developed methodology to other defects in semiconductors that are currently being investigated as viable quantum bits.

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