Modeling Point Defects for Quantum Information Science

Chris G. Van de Walle

Materials Department, University of California, Santa Barbara, California, USA

Defects in wide-band-gap semiconductors have emerged as promising single-photon emitters and solid-state qubits [1]. The nitrogen-vacancy (NV) center in diamond has been widely studied as an individually-addressable quantum system that can be initialized, manipulated, and measured with high fidelity at room temperature. The success of the NV center stems from its nature as a localized "deep-center" point defect. We have performed in-depth first-principles analyses of the NV center in order to elucidate its properties and to predict which centers in other materials might exhibit similarly favorable properties [2, 3, 4]. I will present an overview of the physics of deep centers, focusing on the characteristics that are key to their performance as "NV-like" centers. Building on the general methodology for performing point-defect calculations [5], we have developed the capability to predict transition energies and lineshapes associated with the optical transitions that play a central role in the functionality of the defect. Our methodology rigorously addresses the coupling between electrons and phonons during an optical transition, leading to an excellent description of the luminescence band [6, 7]. We also model nonradiative transitions [8]. The developments will be illustrated with examples for III-Nitride semiconductors including AlN and BN.

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