Modelling the Phonon Coupling of Single Defect Centers in Hexagonal Boron Nitride

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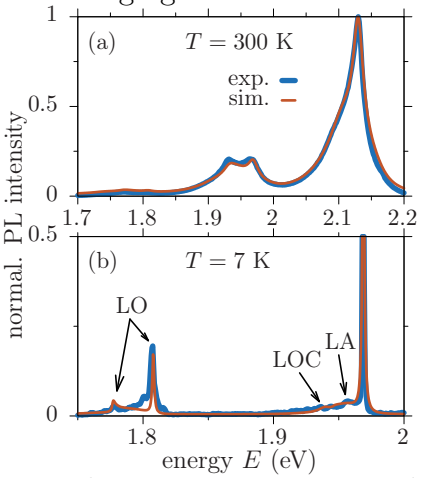
Many quantum applications require reliable single-photon sources. Solid-state light emitters are appealing due to their robustness and promise for scalability. Semiconductor quantum dots, on the one hand, represent a mature technology platform, but presently yield optimum performance only at cryogenic temperatures. Color centers in diamond, on the other hand, show single photon emission at room temperature but suffer from a high refractive index and challenging processability of the host matrix.

Defect centers in hexagonal boron nitride (hBN) [1] stand out as solid-state single-photon sources by combining room-temperature performance and the mechanical flexibility and robustness of layered van der Waals materials. Especially the latter aspect makes this material easy to process and opens many possibilities for implementation. The emitters appear in a wide range of transition energies over the entire visible spectrum. This makes the identification of the underlying atomic structure challenging.



I will present a combined theoretical and experimental study on the phonon coupling of defect centers in hBN[2]. The coupling leads to unique side band emission in photoluminescence and allows for phonon-assisted photon absorption. In photoluminescence spectra, longitudinal optical (LO) phonons lead to strong sideband emission well separated from the zero phonon line (ZPL). In addition, the ZPL itself is asymmetrically broadened, which we attribute to the coupling to longitudinal acoustic (LA) phonons and local oscillation modes of the defect with respect to the bulk crystal. By performing a systematic study based on measurements on 165 different emitters and a theoretical model, we find a correlation between the transition energy and the strength of the LO side bands. This behavior supports the interpretation that the spread of the transition energies is due to the Stark effect induced by nearby trapped charges [3]. From the simulation of the LA phonons we extract reasonable values for the deformation potentials for electrons and holes. As exemplarily shown in the figure, we achieve an excellent agreement between experiment and theory from room temperature down to cryogenic temperatures. In addition, we develop a promising strategy to select a desired ZPL energy from the wide spread of emission energies by exciting the emitter via a LO phonon-assisted photon absorption.

[1] T. T. Tran, K. Bray, et al., *Nat. Nanotech.* **11**, 37–41 (2016).
[2] D. Wigger, R. Schmidt, et al., *resubmitted* (2019).
[3] Z. Shotan, H. Jayakumar, et al., *ACS Photonics* **3**, 2490–2496 (2016).