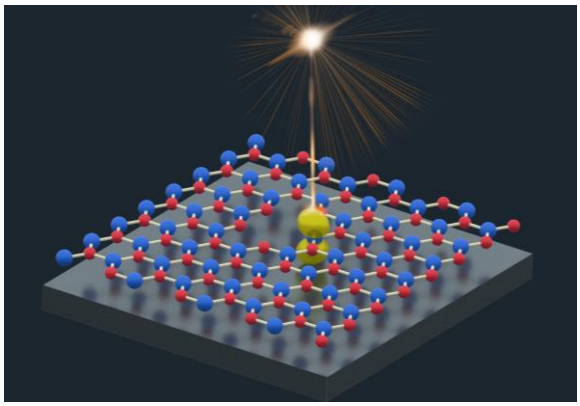
Exploring Properties of Boron Nitride for Quantum Information Science

M. E. Turiansky[a], A. Alkauskas[b], L. C. Bassett[c], and C. G. Van de Walle[d]
[a]Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA
[b]Center for Physical Sciences and Technology (FTMC), Vilnius, LT-10257, Lithuania
[c]Quantum Engineering Laboratory, Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA
[d]Materials Department, University of California, Santa Barbara, CA 93106-5050, USA

Hexagonal boron nitride (h-BN) has been found to host bright single-photon emitters. This emission originates from point defects in the h-BN lattice, and identifying the defects responsible for the emission is of paramount importance for realizing quantum information applications. Using density functional theory, we have identified boron dangling bonds as the likely origin of the single-photon emission near 2 eV [1]. In the negative charge state, boron dangling bonds possess an optical transition at 2.06 eV with minimal coupling to phonons, consistent with experiment. The boron dangling bond also has a metastable triplet state that explains the magnetic field dependence of the emission and can be utilized for spin-based applications. We have also examined the properties of the boron dangling bond in a monolayer of h-BN [2]. Despite the reduced screening, the optical transition is remarkably similar to that in bulk h-BN. However, minor differences in the geometry of the metastable triplet state could lead to differences in the magnetic-field dependence. These results shed light on the single-photon emission in h-BN and provide the opportunity to engineer the properties of h-BN to enhance its suitability for quantum information applications.



Schematic of the boron dangling bond emitting a single photon.

The research reported here was primarily supported by the NSF through the MRSEC at UC Santa Barbara, DMR-1720256 (Seed) and through the Enabling Quantum Leap: Convergent Accelerated Discovery Foundries for Quantum Materials Science, Engineering and Information (Q-AMASE-i) award number DMR-1906325.

References:

1. M. E. Turiansky, A. Alkauskas, L. C. Bassett, and C. G. Van de Walle, Dangling bonds in hexagonal boron nitride as single-photon emitters, *Phys. Rev. Lett.* **123**, 127401 (2019). DOI: 10.1103/PhysRevLett.123.127401
2. M. E. Turiansky and C. G. Van de Walle, Boron dangling bonds in a monolayer of hexagonal boron nitride, *J. Appl. Phys.*, in press (2021).