Unveiling a Unified Mechanism for Single-Photon Emission Across the III-Nitride

Yifeng Cao[1]

[1]*National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA*

Single-photon emission (SPE) is a fundamental phenomenon in future quantum information technologies. As wide-bandgap semiconductors, the III-nitrides —including hexagonal boron nitride (hBN), gallium nitride (GaN), and aluminum nitride (AlN)—have attracted significant interest for its room-temperature operation, strong emission intensity, tunable emission wavelength, and narrow linewidth[1]. However, the origin of SPE in these materials remains largely unknown. Photoluminescence (PL) spectroscopy studies have attributed SPE in nitrides to boron vacancies, gallium antisites, nitrogen vacancies, and other defect states. Yet, none of these mechanisms fully explain the wide range of emission peaks observed in PL data and their spectral wandering. In this study, we applied resonant inelastic X-ray scattering (RIXS) to hBN, GaN, and AlN and identified a series of harmonic peaks with an identical elementary energy of 285 meV across all three nitrides materials [see Figure 1 below]. Using the donor-acceptor pair (DAP) model and comparing with PL data, we determined that these harmonic peaks correspond to SPE features observed in PL. The presence of identical harmonic peaks related to SPE in hBN, GaN, and AlN suggests that SPE in these nitrides is not only linked to their crystal structures but rather our results indicate that molecular N_2 plays a pivotal role in the generation of SPE in these nitrides. This is evidenced by the behavior of the harmonic peaks and their fundamental energy matching a vibronic state of N_2. This discovery highlights the existence of a unified SPE mechanism across III-nitride compounds and suggests that this mechanism could potentially extend to other materials in the III-nitride family. By establishing a common origin for SPE in hBN, GaN, and AlN, this work advances the fundamental understanding of quantum photonics and provides a foundation for future studies on quantum emission phenomena based on molecular-like defects in wide-bandgap semiconductors.

Keywords [optional]: Single photon emission, resonant inelastic X-ray scattering, photoluminescence spectroscopy, wide-bandgap nitrides, N_2 molecule, donor-acceptor model.

[1]Pelliciari, J., Mejia, E., Woods, J.M. *et al.* Elementary excitations of single-photon emitters in hexagonal boron nitride. *Nat. Mater.* **23**, 1230–1236 (2024).

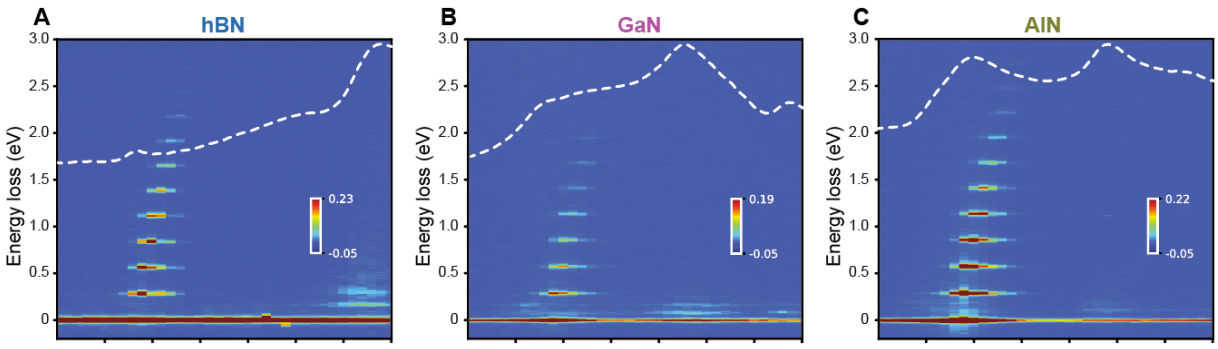

Figure 1: RIXS maps of hBN (A), GaN (B), and AlN (C) at the N-K edge. Harmonic peaks at 285 meV appear at the same incident energy of 401 eV across all three nitrides, while low-energy phonon excitations vary in energy depending on the material. The white dashed lines indicate the X-ray absorption spectroscopy signal.