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(POS-22) Uncovering the Electronic Environment of a Novel Nitridophosphate: GeP2N4

Tuesday 10 June 2025 18:22 (2 minutes)

Characterizing a newly synthesized germanium nitridophosphate, GeP2N4, revealed several interesting aspects of the sample. It is structurally unique to other known MP2N4 systems (M = Be, Ca, Sr, Ba, Mn, Cd) due to the presence of Ge2+ lone pairs that reside within rings of PN4 tetrahedra. Our group makes use of several different techniques to perform these characterizations. Primarily, we perform synchrotron-based X-ray spectroscopy at the REIXS beamline in the Canadian Light Source, probing the electronic states of GeP2N4. More specifically, we find the X-ray emission spectra, X-ray absorption spectra, and X-ray excited optical luminescence. These allow us to determine properties such as the band gap, and make inferences about possible defects, such as vacancies, within our sample. Along with experimental measurements we calculate the entire system using density functional theory in the WIEN2k program. We calculate exactly what we measure, which allows us make direct comparisons between theory and experiment.

Keyword-1

X-ray Spectroscopy

Keyword-2

Density Functional Theory

Keyword-3

Synchrotron

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