

Contribution ID: 214 Type: Poster Competition (Graduate Student) / Compétition affiches (Étudiant(e) 2e ou 3e cycle)

# (POS-14) Band gap and electronic structure of oxygen-containing Ca5Sb2(NH)2: A soft X-ray spectroscopy and DFT

Tuesday 10 June 2025 18:08 (2 minutes)

The air-sensitive Ca5Sb2(NH)2 is studied by soft X-ray absorption spectroscopy (XAS) and emission spectroscopy (XES), which directly probe the partial electronic density of states of the conduction band and valence band, respectively. The density functional theory (DFT) calculations are performed to compare with the measured spectra. The second derivatives of measured N K-edge XES and XAS spectra are used to determine the band gap, which is in good agreement with the calculated band gap using mBJ exchange-correlation potential. The oxygen K-edge XES and XAS spectra are measured to examine the presence of oxygen impurities in the sample. To gain more insight into the structure of Ca5Sb2(NH)2-xOx, DFT calculations are performed for different concentrations of oxygen substitution for nitrogen (4.16, 8.33, and 25%), and it is concluded that the concentration of oxygen impurities lies between 4% and 8% in the sample.

### Keyword-1

Soft X-ray spectroscopy

### Keyword-2

Density Functional Theory

## Keyword-3

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**Session Classification:** DCMMP Poster Session & Student Poster Competition | Session d'affiches DPMCM et concours d'affiches étudiantes (13)

**Track Classification:** Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)