Discovery of a Metastable Photoactive Semiconductor Zn_2SbN_3

Scientific Achievement

Zn_2SbN_3 was theoretically predicted and experimentally synthesized. This material is the first Sb-based nitride and a photoactive semiconductor.

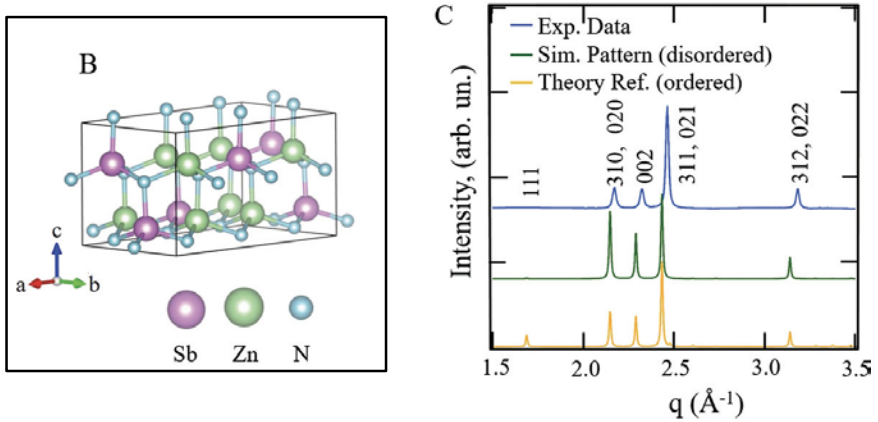
Significance and Impact

No crystalline Sb-based nitrides have been reported so far. The Zn_2SbN_3 reported here crystalized in wurtzite-derived structure and contains Sb in the highest (5+) oxidation state with unusual tetrahedral coordination. It has a solar-matched 1.6–1.7-eV bandgap, band-edge positions matched to water-splitting potentials, and near-band-edge room-temperature photoluminescence, demonstrating its promise as an optoelectronic semiconductor.

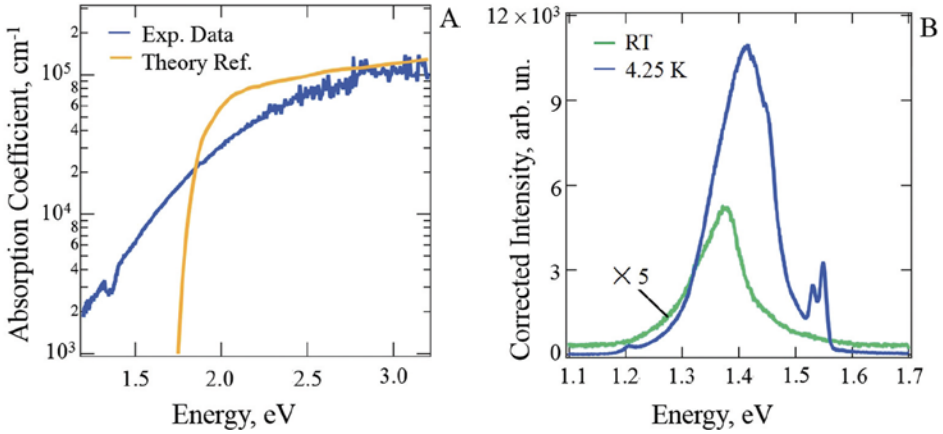
Research Details

Zn_2SbN_3 was identified by theory as a metastable nitride that requires high nitrogen chemical potential. Synthesis from Zn and Sb metallic sources in activated N plasma led to successful synthesis of this new metastable material.

Zn_2SbN_3 Crystalizes in Wurtzite-Derived Structure



Zn_2SbN_3 has 1.7-eV Bandgap and RT Luminescence



E. Arca, J.D. Perkins, S. Lany, A. Mis, B.-R. Chen, P. Dippo, J.L. Partridge, W. Sun, A. Holder, A.C. Tamboli, M.F. Toney, L.T. Schelhas, G. Ceder, W. Tumas, G. Teeter, A. Zakutayev, "Zn_2SbN_3: Growth and characterization of a metastable photoactive semiconductor," *A. Mat. Hor.* (2019), DOI: 10.1039/c9mh00369j

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