

Ternary Nitride Semiconductors in the Rocksalt Crystal Structure

Scientific Achievement

Discovered new class of $Mg_xTM_{1-x}N$ ($TM = Ti, Zr, Hf, Nb$) nitrides that bridges properties and structures found in common nitride materials families.

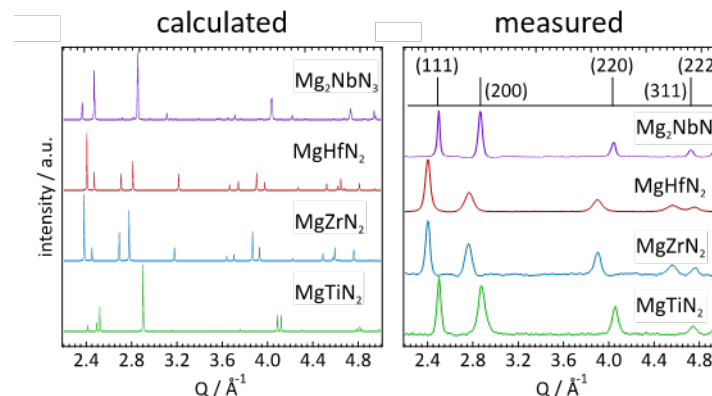
Significance and Impact

Although these materials have rocksalt-derived crystal structures, they exhibit semiconducting band structures, large dielectric constants, and high tolerance to structural defects. Their structural and chemical compatibility with both nitride semiconductors and nitride superconductors make them uniquely poised for epitaxial integration into novel all-nitride devices.

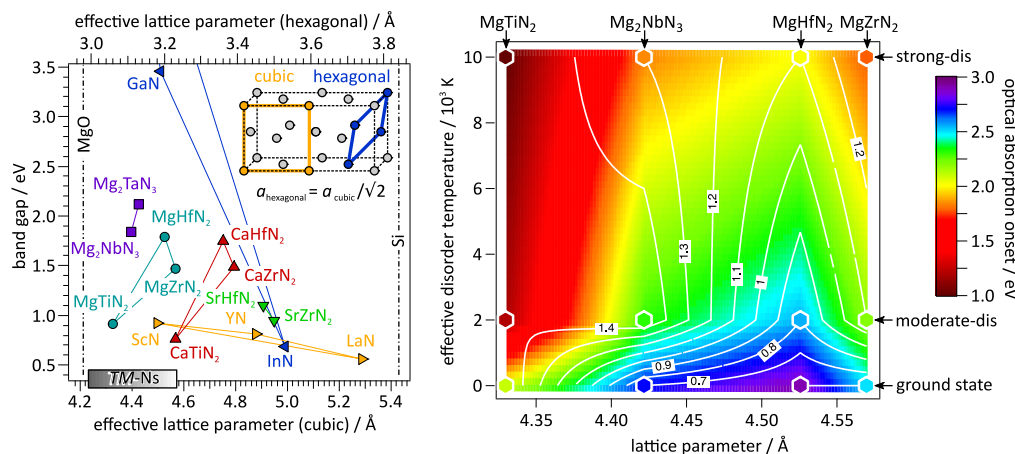
Research Details

Study uses computational stability screening, state-of-the-art structure and properties determination, and high-throughput thin-film synthesis and characterization approaches to theoretically identify and experimentally realize these new materials.

New Defect-Tolerant Materials with Rocksalt-Derived Crystal Structures



Lattice-Matched to Technological Nitrides with Multidimensional Bandgap Tunability



S.R. Bauers, A. Holder, W. Sun, C.L. Melamed, R. Woods-Robinson, J. Mangum, J. Perkins, W. Tumas, B. Gorman, A. Tamboli, G. Ceder, S. Lany, A. Zakutayev, *Proc. Natl. Acad. Sci. U.S.A.*, 2019, DOI: 10.1073/pnas.1904926116.