Exploratory Synthesis: Nitrides

Scientific Achievement

Broadening synthetic capability is a cornerstone of our strategic plan and that of DOE-BES. Under the Argonne Distinguished Postdoctoral Fellowship program, we are launching an exploratory synthesis program in transition-metal nitrides. This program will open new scientific opportunities by delivering new materials for MSD and external collaborators. It will also substantively enhance the synthesis capabilities of MSD to encompass high-temperature, air sensitive chemistries.

The number of nitrides is small because the strength of the nitrogen triple bond places thermodynamic and kinetic restraints on any synthetic route. Our calculations and prior experience in this area show us that both high pressure and flux growth can overcome these obstacles and are ideal techniques to explore transition-metal nitrides.

Significance

Transition-metal oxides present a wealth of crystal structures and properties: high T_c superconductivity, colossal magnetoresistance, relaxor ferroelectricity, etc. Although the number of transition-metal nitrides is much smaller, a relatively large fraction of them exhibit fascinating crystal structures and/or properties. By targeting nitride analogues of oxides we expect to explore the similarities and differences between the members of both systems as well as to discover new transition-metal nitrides structures with compelling properties.

Performers

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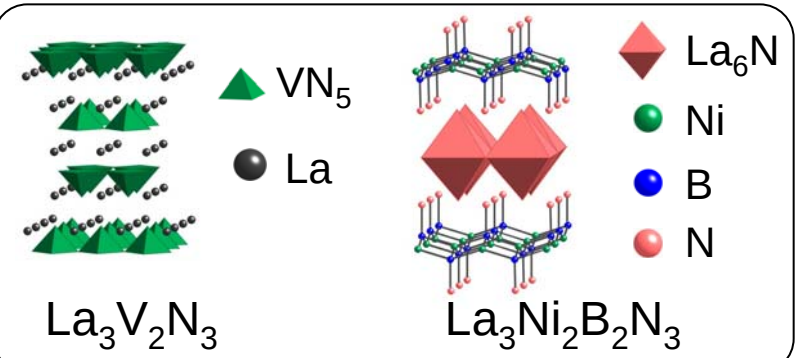
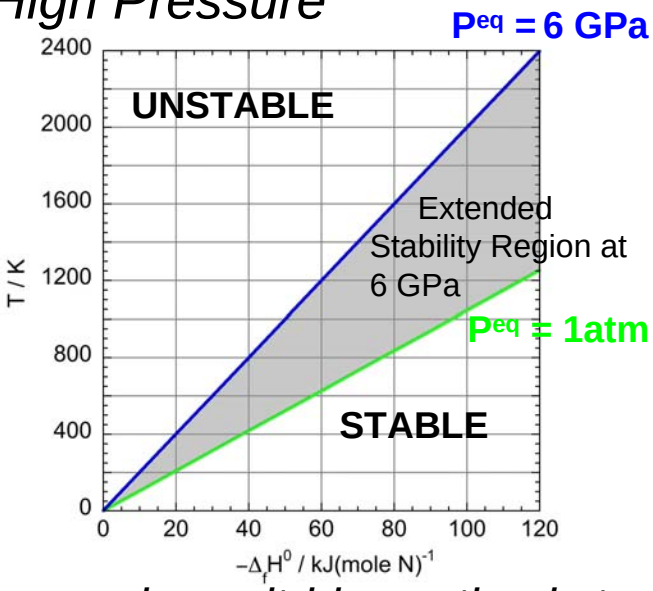
New materials present an opportunity for breakthrough advances in properties.

$La_3V_2N_5$ and $La_3Ni_2B_2N_3$ have compelling crystal structures. However, both nitrides and boron-nitrides are rare.



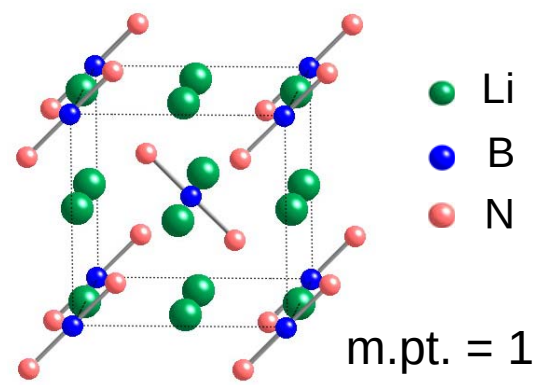
We intend to explore nitrides with suitable experimental techniques

Nitrides: High Pressure



High Pressure raises nitride synthesis temperatures.

Boron-Nitrides: Flux Growth



m.pt. = 1189 K

Li_3BN_2 may be an ideal flux for complex boron-nitrides.

ANL-MSD authors
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