Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides

Scientific Achievement

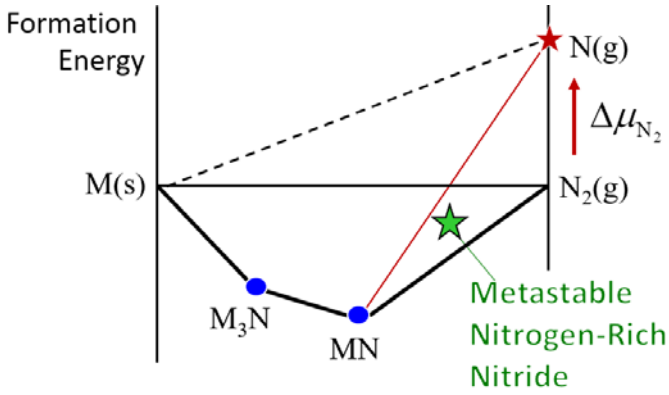
We formulate how reactive nitrogen precursors (e.g., cracked N_2, NH_3) can stabilize metastable nitrogen-rich nitrides during synthesis. With this synthesis strategy, we use density functional theory to predict 22 new nitrogen-rich binary nitrides stabilizable under $\Delta\mu N_2$ = +1 eV/N.

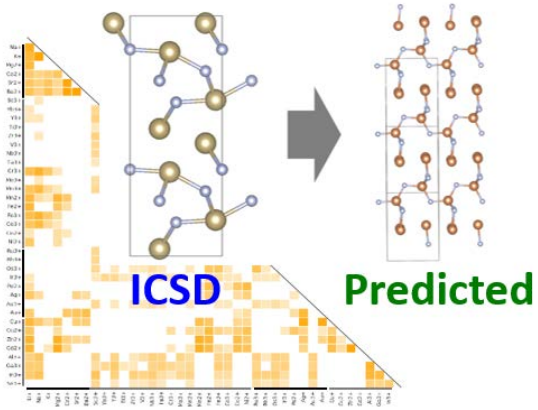
Significance and Impact

Nitrogen-rich nitrides can possess useful semiconducting properties for optoelectronic applications, but are generally metastable. By formulating rational thermodynamic routes to metastable compounds, we expand the search space for functional technological materials beyond equilibrium phases and compositions.

Research Details

- We trained a data-mined ionic substitution algorithm for nitride discovery, cross-validated to achieve 80% "recovery" rate.
- 1,500 candidate binary nitrides were generated by substitution algorithm; phase stability was then evaluated with DFT-SCAN.
- We identify novel stabilizable nitrogen-rich nitrides in 15 X-N chemical spaces:
  X = {Au, Bi, Cr, Fe, Ir, Mn, Mo, Re, Se, S, Sb, Sn, Te, Ti, V}





Notable new stabilizable nitrides

Mn_3N_4 **Cr_3N_4** **V_3N_4** **Nb_3N_5** **SbN**

High-pressure "pernitrides" **FeN_2, CrN_2**

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Chemistry of Materials **29**(16), 6936–6946 (2017).

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