Design of Nitride Semiconductors for Solar Energy Conversion

Scientific Achievement

A new perspective on the promising properties, unexplored chemistry, and metastable character of nitride semiconductors for solar energy conversion.

Significance and Impact

Nitrides have promising semiconductor properties for solar energy conversion (Fig. 1), but are much less studied than oxides, in part, because many are metastable. However, they can often be synthesized using high-energy N-atom precursors and nonequilibrium growth methods (Fig. 2).

Research Details

Promising Properties: Higher energy of nitrogen 2p orbitals leads to narrower bandgaps and more disperse energy bands.

- **Unexplored Chemistry:** Nitrides are much less explored compared to oxides (1:14 ratio of Nitrides:Oxides in ICSD).
- **Metastable Character:** Despite apparent metastability with respect to low-energy N₂ molecule (-10 eV), nitrides can be synthesized using reactive N-atom precursors (N, NH₃, MN₃).

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Fig. 1: Schematic electronic structure of oxides vs. nitrides



Fig. 2: Generalized energy landscape for nitride synthesis



