Exploration of Novel Nitride Semiconductors by *In Silico* Screening and Experimental Verification

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The exploration of novel functional materials is increasingly important as the demands for earth-abundant, environmentally benign, and low-cost materials grow in various fields. The materials search solely by experiment, however, requires tremendous efforts and this fact largely limits the search space. In this study, we developed first-principles methods for *in silico* high-throughput screening of semiconductors to overcome this difficulty in the materials search. Novel nitride semiconductors were explored using these methods and the most promising system among those identified was considered as a target of experiment.

The *in silico* screening identified 11 as-yet-unreported nitrides that are thermodynamically stable or slightly metastable and have favorable electronic properties. Among them, the most promising system is $CaZn_2N_2$ that is composed of abundant elements only, and has a direct gap of 1.8 eV and carrier effective masses smaller than GaN (Fig. 1). Using high-pressure synthesis at 1200 °C and 5.0 GPa for 1 hour, this novel phase is obtained with a predicted trigonal crystal structure. The experimental band gap of 1.9 eV is close to the theoretically predicted value. Moreover, band-edge red photoluminescence is observed as shown in Fig. 1, indicating its direct-type band structure. These results demonstrate accelerated materials discovery via *in silico* screening followed by targeted experiments.

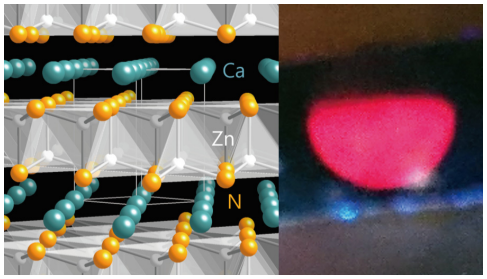

Fig. 1. Crystal structure of $CaZn_2N_2$ identified via *in silico* screening using first-principles calculations and experimental verification of band-edge red photoluminescence from $CaZn_2N_2$.

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