Computational Design and Exploration of Novel Semiconductors

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The search for novel semiconductors is increasingly important as the applications of semiconductors become more prevalent. Among the compound semiconductors, nitrides are attractive due to the abundant and environmentally-benign nitrogen constituent. Currently commercialized nitride semiconductors are, however, mostly limited to GaN and its based alloys. This situation stimulates not only experimental but also computational, or *in silico*, exploration of novel nitrides. In this talk, we report the discovery of a novel nitride semiconductor $CaZn_2N_2$ by *in silico* screening using first-principles calculations followed by high-pressure synthesis [1], as well as our computational methods for the screening [2,3].

The *in silico* screening identified 11 as-yet-unreported nitrides that are thermodynamically stable or slightly metastable and have favorable electronic properties [1]. Among them, the most promising system is $CaZn_2N_2$ that is composed of abundant elements only, and has a direct-type band structure with a gap of 1.8 eV and carrier effective masses smaller than GaN (Fig. 1). The native defect and dopant calculations indicate that this compound is dopable into both *p*- and *n*-types. We therefore choose $CaZn_2N_2$ as a target of experiment. 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.

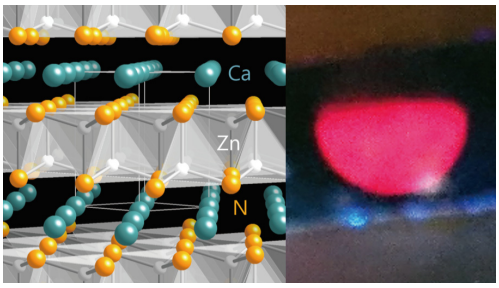

Fig. 1. Crystal structure of $CaZn_2N_2$ identified via *in silico* screening and experimental verification of band-edge red photoluminescence.

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[1] Y. Hinuma, T. Hatakeyama, Y. Kumagai, L. A. Burton, H. Sato, Y. Muraba, S. Iimura, H. Hiramatsu, I. Tanaka, H. Hosono, and F. Oba, *Nat. Commun.* **7**, 11962 (2016).
[2] Y. Kumagai and F. Oba, *Phys. Rev. B* **89**, 195205 (2014).
[3] Y. Hinuma, Y. Kumagai, I. Tanaka, and F. Oba, *Phys. Rev. B* **95**, 075302 (2017).