Oba-Kumagai Lab

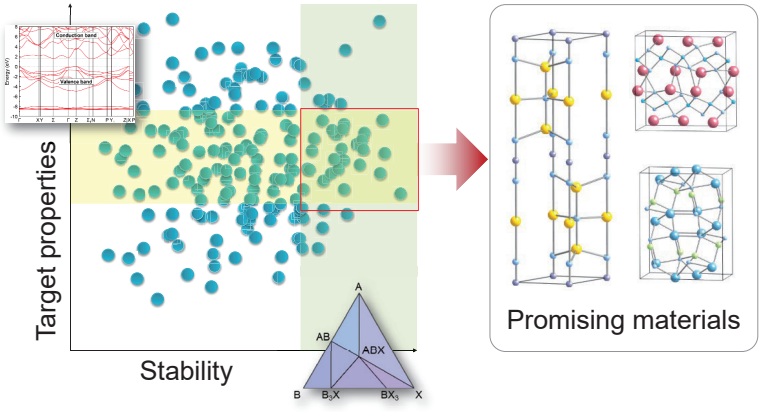
Computational Materials Design

Laboratory for Materials and Structures

http://www.msl.titech.ac.jp/~oba

- **Design and exploration of electronic materials**
- **Computational materials science and materials informatics**

It is now feasible to predict a variety of the structure and functionalities of materials using computer simulations at the practical level of accuracy required for detailed understanding and elaborate design of materials, thanks to recent development of relevant theory and methodologies along with computer performance. Our aim is to design and explore novel inorganic materials, particularly semiconductors and dielectrics, using approaches based on computational and data science.

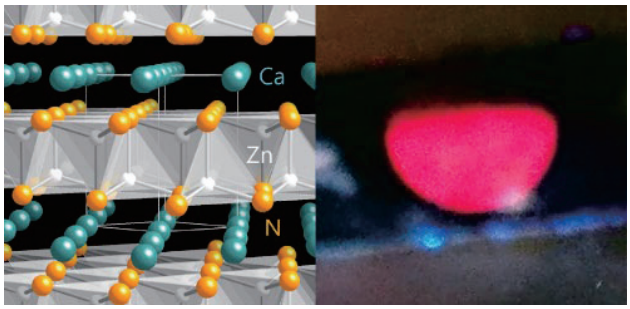


Materials exploration by high-throughput computational screening

- Prediction of material properties and stability using first-principles calculations and machine-learned prediction models
- Identification of promising materials in terms of target properties and stability by high-throughput computational screening

Development of computational methods for materials exploration

- High-throughput first-principles calculations
- Machine learning of calculation data



Successful example of computational materials exploration: Discovery of a novel nitride semiconductor

- Prediction of $CaZn_2N_2$ with a band structure suited for red light emission
- Experimental verification of the predicted crystal structure and optical properties (Hosono-Hiramatsu group)

Hinuma *et al.*, *Nat. Commun.* **7**, 11962 (2016).