

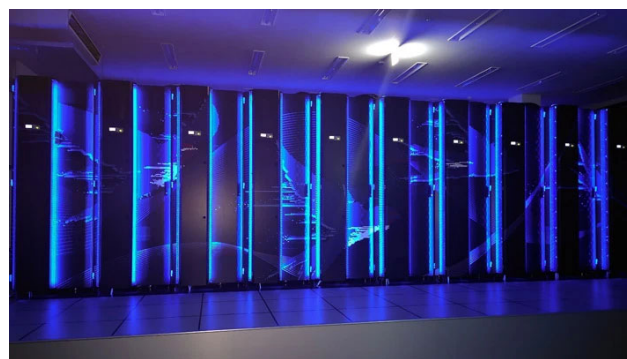
Computational Material Design

Laboratory for Materials and Structures

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

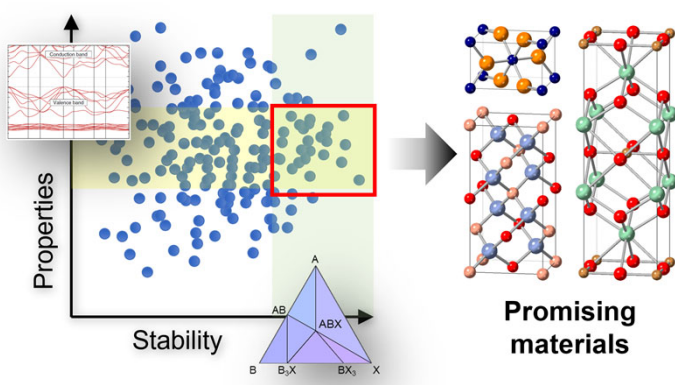
- Design and exploration of electronic materials
- Computational materials science and materials informatics

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.



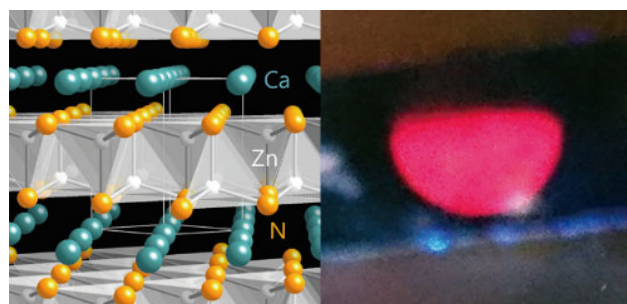
Development of computational methods for material exploration

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



Material 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



Successful example of computational material 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).