



## Computational Materials Design

Laboratory for Materials and Structures

[www.cms-mi.msl.titech.ac.jp](http://www.cms-mi.msl.titech.ac.jp)

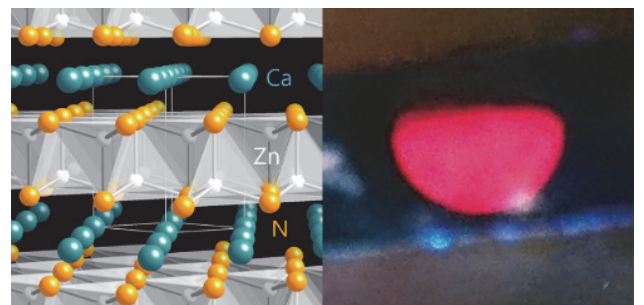
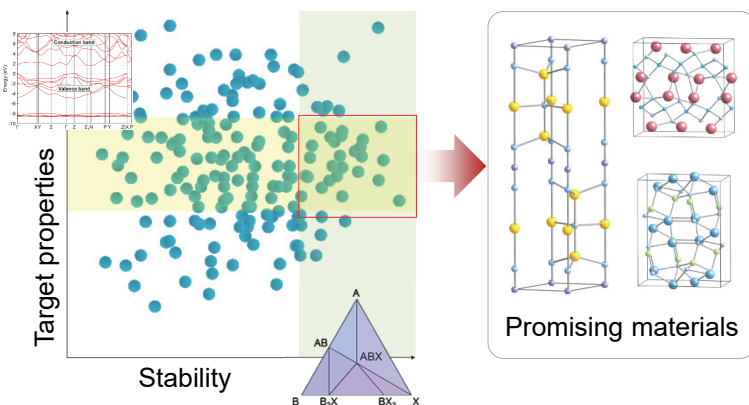
- Design and exploration of electronic materials
- Computational materials science and materials informatics

It is now feasible to predict a variety of structures and functionalities of materials using computer simulations at the practical level of accuracy required for detailed understanding and elaborate design of materials, thanks to the recent development of relevant methodologies and 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 materials exploration

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



### Materials exploration by high-throughput computational screening

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

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

- Prediction of  $\text{CaZn}_2\text{N}_2$  with a band structure suited for red light emission
- Experimental verification of the predicted crystal structure and optical properties (Hosono and Hiramatsu groups)

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