

Development of unexplored materials accelerated by ab initio calculations and informatics

Keywords: Materials exploration, Epitaxial thin film growth, ab initio calculation, Materials informatics, Thermoelectric materials

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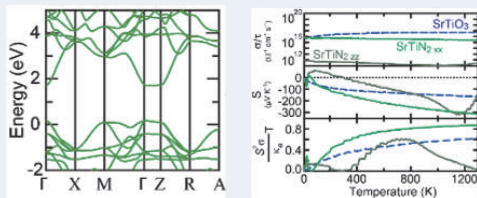


Background Materials design and selection based on ab initio calculation, materials informatics, machine learning have led to unprecedented capabilities for materials discovery and development. In this study, to promote innovations in the research field of materials science, advantages of materials design, screening and synthesis using above mentioned materials informatics techniques in the development of unexplored materials are revealed.

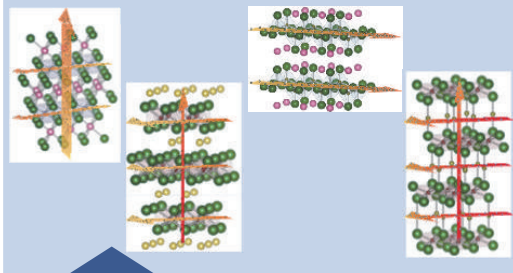
- Aim**
- Establishment of synthesis techniques of unexplored materials using epitaxial growth techniques
 - Predictions of physical properties and electronic structures of unexplored materials by density functional theory (DFT) calculations
 - Development of efficient synthesis parameters optimization using machine learning method

Advanced Research Topics

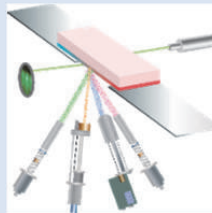
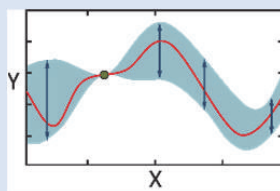
Materials selection using ab initio calculations and informatics



Development of unexplored materials



Efficient materials synthesis using machine learning method



Publications [1] I. Ohkubo and T. Mori, *Chem. Mater.* **26**, 2532 (2014). [2] I. Ohkubo and T. Mori, *Inorg. Chem.* **53**, 8979 (2014). [3] I. Ohkubo and T. Mori, *Eur. J. Inorg. Chem.* 3715 (2015). [4] I. Ohkubo and T. Mori, *Chem. Mater.* **27**, 7265 (2015). [5] I. Ohkubo and T. Mori, *APL Mater.* **4**, 10480 (2016). [6] I. Ohkubo and T. Mori, *J. Phys. Soc. Jpn.* **86**, 074705 (2017).

Applied area and future prospects

- Predictions of thermoelectric transport properties and electronic structures of unexplored materials by DFT calculations
- Development of new epitaxial growth techniques for exploration of undeveloped materials

Issues for technology transfer

- Development of new functional materials among the unexplored materials
- Establishment of synthesis technique of unexplored materials using epitaxial growth technique