Development of unexplored materials accelerated by first-principles calculation and informatics

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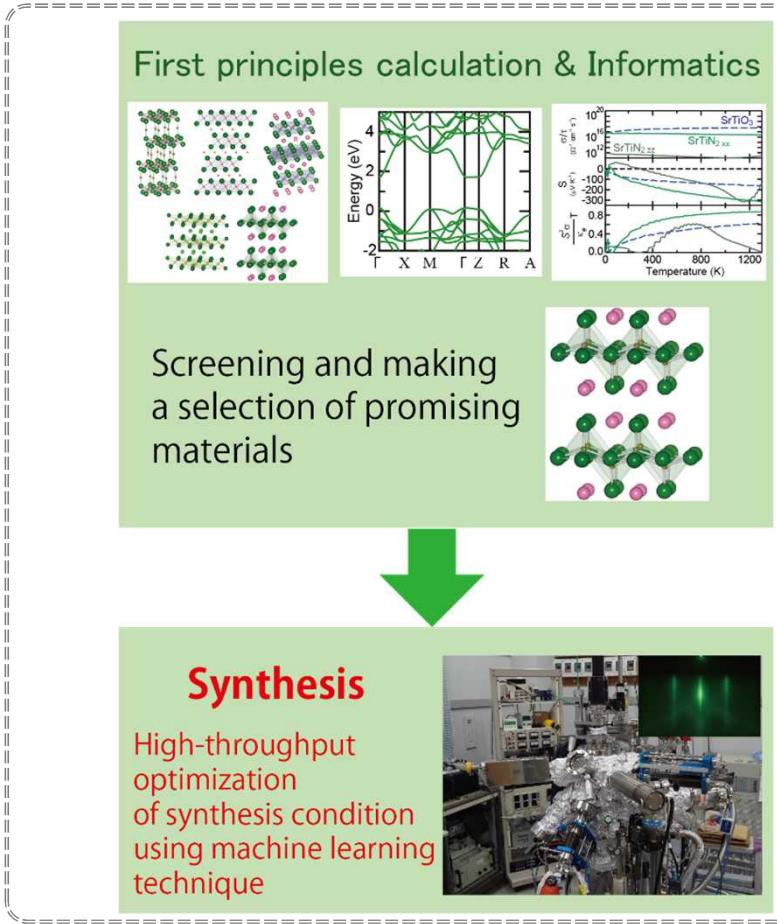
Isao Ohkubo（National Institute for Materials Science, Senior Researcher)

Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

Recent technical advances in the area of first-principles calculation and materials informatics have led to unprecedented capabilities for materials discovery and development. Screening and making a selection of materials by first-principles calculation and informatics are accelerating the materials discovery and development. Among the undeveloped material groups, layered complex nitrides are of interest because remarkable physical properties have been predicted. Exploration of undeveloped materials using first principles calculation, machine learning and thin film growth techniques is carried out.



Achievement

The contents of this study are as follows.

- Prediction of electronic strictures and physical properties of layered complex nitrides using density functional theory calculation
- Development of a new thin film growth technique for synthesis of layered complex nitrides
- High-throughput optimization of synthesis condition using machine learning technique

Reference/Link

[1] I. Ohkubo and T. Mori, *APL Mater.* 4, 104808-1～104808-5 (2016).
[2] I. Ohkubo and T. Mori, *J. Phys. Soc. Jpn.* 86, 074705-1～074705-7 (2017).
[3] https://samurai.nims.go.jp/profiles/ohkubo_isao?locale=ja