

## 4<sup>th</sup> International Symposium on the Frontiers of Functional Materials Research

Date & Time: 10:00 – 17: 10, Jun 19<sup>th</sup>, 2024

Place: Meeting Room, South Multidisciplinary Research Laboratory 2  
IMRAM, Katahira campus, Tohoku University  
[https://www.tohoku.ac.jp/map/en/?f=KH\\_E03](https://www.tohoku.ac.jp/map/en/?f=KH_E03)

It is easy to make bad devices out of good materials but impossible to make good devices with bad materials. Materials always come first. This symposium invites the world's leading scientists to discuss state-of-the-art research on functional materials for, e.g., batteries, solar cells, thermoelectrics, fuel cells, ferroelectrics, and other energy-related materials.

This time, we have a guest speaker, Prof. Prashun Gorai from Colorado School of Mines (USA), to discuss recent topics in the computational approach to searching and designing new functional materials and provide an opportunity to exchange research ideas and perspectives with young researchers and students at Tohoku University. Furthermore, front-running researchers in Japan are getting together to exchange ideas and opinions on cutting-edge research on Functional Materials.

### Time table

- 10:00 – 10:05 Opening remarks (Saneyuki Ohno)
- 10:05 – 10:45 **Dr. Hirofumi Akamatsu (Kyushu Univ.)**  
“Experimental and theoretical studies on non-oxide polar materials”
- 10:45 – 11:25 **Dr. Akira Nasu (Hokkaido Univ.)**  
“Proposal of a Novel Synthesis Route Using Na<sub>2</sub>S<sub>x</sub> Reaction Medium for Sodium Solid Electrolytes”
- 11:25 – 12:05 **Dr. Marcela Calpa (NIMS)**  
“Liquid-phase synthesis of sulfide solid electrolytes”
- Lunch break (at the venue)---
- 13:00 – 13:40 **Dr. Prashun Gorai (Colorado School of Mines)**  
“Emerging Materials, Mechanisms, and Design Principles for Wurtzite-type Ferroelectrics”
- 13:40 – 14:20 **Dr. Saneyuki Ohno (IMRAM, Tohoku Univ.)**  
“Exploration of new classes of inorganic ion conductors”
- Coffee break---
- 14:40 – 15:20 **Dr. Akira Miura (Hokkaido Univ.)**  
“Metastability: what it is? how it works?”
- 15:20 – 16:00 **Dr. Masaya Fujioka (AIST)**  
“Synthesis strategy for metastable materials”
- 16:00 – 16:40 **Dr. Tetsuya Yamada (Shinshu University)**  
“Application of data-driven and autonomous robotics techniques to materials research based on flux crystal growths”
- 16:40 – 17:10 **General discussion (+Lab tour)**
- 18:30 – Reception and discussion (Move to Sendai station)
- 20:00 – 21:00 Extended discussion



**Prashun Gorai:** My research focuses on discovery and design of novel materials for functional applications and development of composition-structure-property heuristics that enable *materials by design*. As we balance societal growth with rising energy needs and climate challenges, our progress is predicated on discovering and engineering materials for advanced technologies. Historically, materials have been discovered by Edisonian trial-and-error approaches and even serendipitous “happy accidents”. Designing materials with tailored properties is challenging because of the astronomical number of possible compounds, structures, and morphologies. In the last decade, computational chemistry has made great strides in accelerating materials development, but many unexplored avenues and long-standing bottlenecks remain. We are addressing some of these challenges, including inverse design of materials in large unexplored chemical spaces, systematic optimization of materials to improve performance, and prediction of properties to bridge the gap between idealized theoretical predictions and real materials. My research program utilizes first-principles computational methods and machine learning to address these materials challenges. In this talk, I will share examples from our work on discovery and design of materials for thermoelectrics, photovoltaics, and solid-state energy storage. I will also share our work on predictive defect modeling for defect engineering of functional materials.

**Contact:**

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