

Title**From Atoms to Applications:
Computational Discovery and Design of Functional
Materials****Speaker****Assistant Professor Prashun Gorai**Chemical & Biological Engineering, Rensselaer Polytechnic Institute,
Troy, NY**Time & Date**

2:00 PM (JST), Tuesday, May 26th, 2026

VenueI²CNER Hall C, I²CNER Bldg. 1, Ito Campus**This seminar will be held on-site only. Please note there are no online or hybrid sessions.***Abstract**

Technological developments often rely on specifically designed materials and molecules. The increasing pace of technology development, coupled with rising energy needs and climate challenges, requires faster approaches for materials discovery. Historically, materials have been discovered by trial-and-error approaches that rely on chemical intuition. Designing materials with tailored properties is challenging because of the astronomical number of possible compounds and structures, and materials behaviors that do not adhere to standard chemical intuition. In this talk, I will share examples from our work on the computational discovery and design of functional materials, specifically focusing on wurtzite ferroelectrics for energy-efficient data storage and inorganic solid electrolytes for energy storage. We employ first-principles computations, high-throughput computing, and machine learning in close collaboration with experiments to discover novel materials and generate new materials design principles, with the goal to accelerate materials discovery and guide experimental realization.

About the Speaker

Dr. Prashun Gorai is an Assistant Professor in Chemical & Biological Engineering at the Rensselaer Polytechnic Institute. He received his bachelor's degree from IIT Madras (India) and his PhD from the University of Illinois at Urbana-Champaign. He was a postdoctoral fellow at the Colorado School of Mines and National Renewable Energy Laboratory. Dr. Gorai was previously a Research Assistant Professor at Mines. He uses quantum-chemical calculations, high-throughput computing, and machine learning to discover and design functional materials for energy and microelectronics. The International Thermoelectric Society awarded him the Young Investigator Award in 2022, and Materials Horizons (RSC) and ACS Materials Letters (ACS) have recognized him as an Emerging Investigator. He is a recipient of the Chemistry of Materials Lectureship and Best Paper Award 2023. In 2025, he received the American Chemical Society PRF Doctoral New Investigator Award.

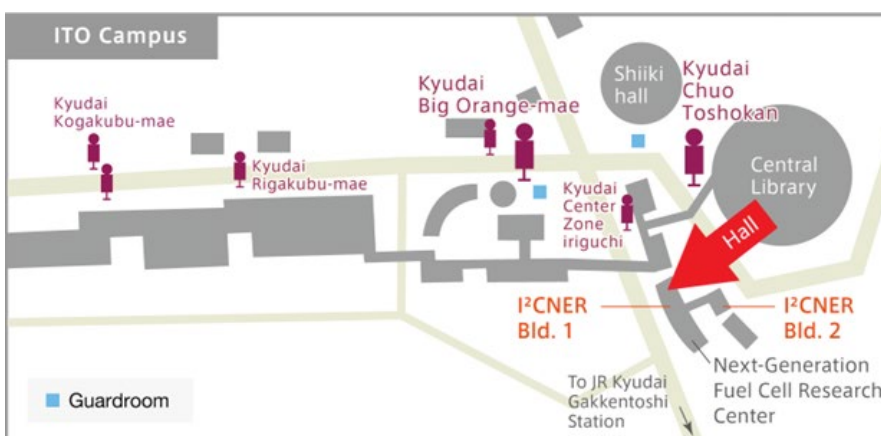
Registration<https://forms.cloud.microsoft/r/dSQVVUcMXD>**Host**

Prof. Aleksandar Staykov

ContactI²CNER · Q-PIT Office of Research Support Services,

Research Support and Public Relations

Tel.: +81 92 802-6935 Email: iq-kenkyu@jimu.kyushu-u.ac.jp

Register
here!!