Dr. Kartik Sau

Specially Appointed Senior Assistant Professor (**Ph.D.**)

- Place: Sendai, Japan
- Nationality: **Indian**
- Date of Birth: January 27, 1989
- Married

Core Skills

Machine Learning, DFT

Softwares (VASP, LAMMPS, OVITO, VMD, VESTA, Blender)

Programming (C, Fortran, Python)

Team Management and Leadership 11+ Yrs

Cloud computing (Azure) 3+ yrs.

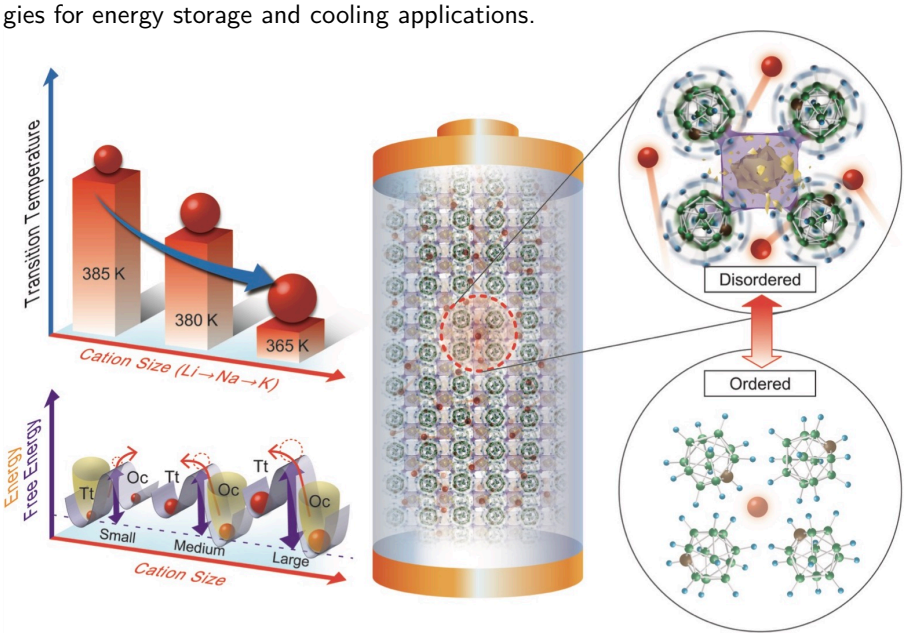
Operating System Windows, Linux, Mac

English Business Level

Japanses Basic Level

Professional Summary

Research experience with 8+ years in force-field based, first-principles and machine-learning-accelerated molecular dynamics applied to solid-state battery electrolytes and hydrogen storage materials. Track record of >25 peer-reviewed papers, >10 M JPY in funded projects, and cross-functional team leadership. Proven ability to translate atomic-level insights into commercialisable technologies for energy storage and cooling applications.



I am enthusiastic about tackling new challenges and working in a team.

Professional Experience (Eight years)

Specially Appointed Senior Assistant Professor — **4/2024 - today**

AIMR, Tohoku University, **Sendai** 980-8577, **Japan**

Research Theme: **Computer simulation studies in fast ion conductors and hydrogen storage materials.**
Here, I studied several complex hydrides using MD for battery electrolytes for all-solid-state battery and hydrogen storage applications.

Post-Doctoral Research — **11/2023 - 3/2024**

AIST-MathAM-OIL, c/o AIMR, Tohoku University, **Sendai** 980-8577, **Japan**

Research Theme: **Molecular dynamics simulations in fast ion conductors and hydrogen storage materials.**

JSPS Post-Doctoral Research — **11/2021 - 10/2023**

AIMR, **Tohoku University, Japan**

Research Theme: **Designing principles and guidelines of fast ion conductors for ASSB electrolyte.**
In this project, I perform MD simulation studies on complex hydrides, an excellent fast ion conductor.

Education

06/2011 - 06/2017

Computational Condensed Matter Physics (Ph.D.)

Indian Institute of Technology Guwahati, **India**

Condensed Matter Computational Ph.D. thesis: Modeling and Simulation of Fast Ion Transport in Oxide Frameworks.

06/2009 - 06/2011

Physics (M.Sc.)

Indian Institute of Technology Guwahati, **India**

Condensed Matter Statistical Mechanics

Master's thesis: Molecular Dynamics study of Ionic Motion in AgI.

07/2006 - 06/2009

Physics (B.Sc.)

University of Calcutta, **India**

Physics (major) Chemistry Mathematics .

Interests

- Fitness (gym, cycling, skating, skiing, etc.)
- Sketching
- Travel

Contact

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Google Scholar

Post-Doctoral Research, AIST Kansai — **06/2021 - 10/2021**

Advanced Battery Research Group Ikeda, **Osaka, Japan**

Research Theme: **Theoretical simulations in honeycomb layered oxides for high voltage batteries.**
Here, I studied several honeycomb layered oxides for battery applications using theoretical simulation. The main goal was to find suitable and low-cost advanced materials for the high-voltage battery. We also found that mixed ion conducting (Na and K) materials show a lot of promise.

Post-Doctoral Research — **07/2017 - 06/2021**

AIST-MathAM-OIL, c/o AIMR, Tohoku University, 2-1-1 Katahira, Aoba, **Sendai** 980-8577, **Japan**

Research Theme: **Molecular dynamics simulations in fast ion conductors.**
Here, I studied several complex hydrides and Na-super ionic conductors (NASICON) using MD for battery electrolytes for all-solid-state battery applications.

Collaborative Research — **07/2017 - Continue**

Taiwan, Spain, Australia.

I studied advanced functionality in complex hydrides (baro-caloric effect for solid-state cooling application) using MD simulation.

Country Traveled

America, Australia (two times)

I traveled for my research work, such as attending conferences and also for research collaborations.

Highlighted Publications (25+ ...)

- **Sau, K.***, .., and Orimo, S., Comparative Molecular Dynamics Study of the Roles of Anion-Cation and Cation-Cation Correlation in Cation Diffusion in $Li_2B_{12}H_{12}$ and $LiCB_{11}H_{12}$. **Chemistry of Materials** 33, 235769 (2021).
- Masese, T., , **Sau, K**. Mixed alkali-ion transport and storage in atomic-disordered honeycomb layered $NaKNi_2TeO_6$, **Nature Communication**, (2021).
- **Sau, K.** et al. Colossal barocaloric effects in the complex hydride $Li_2B_{12}H_{12}$. **Scientific Reports** 11, 11915 (2021).

Achievements

- **Funded Project Budgets**: I completed several projects (AIST MathAM-OIL (**8.8 million yen**) and Fusion Research Project two times (**2 million yen**).
- **Awards**:1. **Certificate of Commendation from the President of Tohoku University** for a lifesaving activity (link). 2. **Certificate of appreciation from Sendai Police** for a lifesaving activity. 3. My research figure was selected for the IMR supercomputer (Tohoku University) news cover page.

Sendai, August 5, 2025 _____