CCMS

Center for Computational Materials Science
Institute for Materials Research
Tohoku University

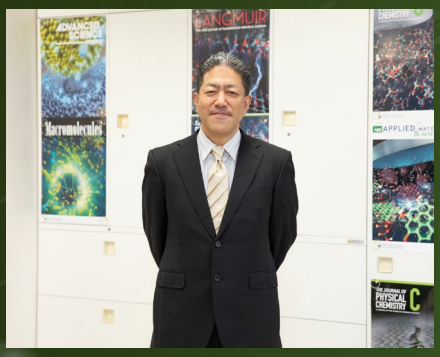


MASAMUNE-弐

MAterials science Supercomputing system for Advanced MUlti-scale simulations towards NExt-generation II

Greetings

Head, Momoji KUBO



Great expectations towards the computational science, data science, and AI-driven science have been growing and growing in recent years in order to achieve the future societies that humanity strives for, such as creating a prosperous and livable societies with well-being, achieving carbon neutrality to suppress global warming and extreme weather, building resilient nations that protect human lives and recovers quickly from large-scale disasters, and developing Society 5.0 which integrates cyber and physical spaces to promote economic development and resolve social issues.

Currently, “Next-Generation Computational Science Global Reach & Innovation Program”, administrated by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), is being pursued to promote the strategic development of application software that leverages Japan’s flagship supercomputer “Fugaku” and other high-performance supercomputers, while addressing emerging technological trends such as the integration of simulations and AI. This Center for Computational Materials Science (CCMS) is organizing one of the projects under this program; “AI-Driven Computational Materials Science Exploration and Materials Co-Innovation (AICoMS)” (Project Leader: Momoji Kubo, FY2026 - FY2030). This project is running by a team of around 150 people divided into five subgroups: Sub-project A: Structural Materials, B: Magnetic Materials, C: Electrochemical Materials, D: Electronics Materials, and E: Bio-Polymer Materials. Particularly, innovative technologies for integrating simulations and AI, based on large-scale, long-time, and massive calculations which can only be realized by supercomputer “Fugaku” and other high-performance supercomputers, are being developed.

The supercomputing system of CCMS is positioned in the second tier of Japan's computing resource hierarchy, directly connected to the flagship supercomputer “Fugaku”, and is expected to make a significant contribution to the advancement and promotion of materials science. In June 2025, CCMS started operating a new supercomputing system called “MASAMUNE-II”, consisting mainly of HPE Cray XD220v and HPE Cray XD670 systems. Compared to the previous system, the computing performance has been enhanced to 4.6 PFLOPS, and it consists of three systems tailored to user’s needs. As an international collaborative research institute, CCMS provides supercomputer computing resources not only to the Japanese materials science community but also to the overseas users. CCMS also promotes the development of application software for supercomputers and their application to materials science. Our aim is to advance creative and innovative research, contributing materials science field as a leading supercomputer center with high originality and creativity. We would appreciate your continuous support and cooperation with CCMS.

Supercomputing System for Computational Materials Science

The high-performance supercomputing system of CCMS specializes in materials science simulations and can satisfy diverse needs in computational materials science research. It consists mainly of HPE Cray XD220v and HPE Cray XD670 with GPU accelerator, and its total theoretical peak performance is 4.6 PFLOPS. This system provides the domestic and foreign researchers in the field of materials science with various application software for materials design.

Mission of Center for Computational Materials Science (CCMS)

Since the first introduction of the supercomputing system in 1994, CCMS has renovated the supercomputing system five times, and it has been used by the researchers of materials science field as a collaborative research hub in the Institute for Materials Research (IMR). In 2009, CCMS established frameworks as a domestic collaborative research institute and has contributed to producing a wide variety of creative and innovative achievements in materials science field by providing computational resources to materials science researchers. Furthermore, in 2018, CCMS was certified as an international collaborative research institute.

The system renovation in 2025 and system enhancement in 2026 make it possible to provide new computational resources which satisfy diverse research needs such as "Multi-Scale Simulations", many-core-server based "Super-Large Scale Parallel Computing", and GPU-based “AI for Science”, in addition to the conventional demands such as prediction of physical phenomena and materials design. This renovation aims at contributing to the creation of a well-being society as the future vision of humanity, as well as the realization of carbon neutrality, resilient nations, and Society 5.0. CCMS also hopes to contribute to advancing the computational materials science field and community in the world by disseminating leading-edge research outcomes obtained by the maximum utilization of our supercomputing system.

Furthermore, CCMS also organizes “Professional development Consortium for Computational Materials Scientists (PCoMS)” for developing young professionals and “Computational Materials Science Forum (CMSF)” for providing active supports for the promotion of computational materials science community.



Supercomputing system

Total Theoretical Peak Performance of Suptecomputer : 4.603 PFLOPS*1

Supercomputer

HPE Cray XD220v

Total Nodes	127 nodes
Total Theoretical Peak Performance	0.910 PFLOPS
Total Memory Size	74.0 TiB*2

HPE Scale-up Server 3200

Total Nodes	2 nodes
Total Theoretical Peak Performance	0.116 PFLOPS
Total Memory Size	8.0 TiB

HPE Cray XD670

Total Nodes	13 nodes
Total Theoretical Peak Performance	3.577 PFLOPS
CPU	0.093 PFLOPS
GPU	3.484 PFLOPS
Total Memory Size	13.0 TiB



Storage System

DDN EXAScaler ES400NVX2

Total Disk Capacity	5.07 PB

*1: FLOPS is a unit representing the number of operations that can be performed per second. 1 PFLOPS means 10^{15} operations per second.
*2: 1 TiB = 2^{40} byte

Nickname and Front Panel Design of Supercomputing System

MASAMUNE-弐
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Nickname “MASAMUNE-II” has been given to the supercomputing system of CCMS, continuing the nickname of the previous system “MASAMUNE-IMR”, in honor of “Masamune Date”, the first lord of Sendai in the 17th century, who dispatched the sailing ship “San Juan Bautista” towards the world from Sendai in 1613. The nickname “MASAMUNE-II” expresses our hope that creative and innovative achievements of the advanced multi-scale simulations on materials science by our supercomputing system will give great impacts towards the next-generation from Sendai to the world. “Masamune Date” is drew on the front panel of our supercomputer by Sumi-E Artist OKAZU with the brave letter “弐” meaning “second” in Japanese Kanji. This “Masamune Date” on the front panel is looking ahead to the future advances in the materials science of the world from Sendai.

Simulation Results by IMR Supercomputing System

01

Elucidation of Effect of Environments on Wear Phenomena of Diamond-like Carbon and Proposal of Design Principles towards Improving its Durability

Diamond-like carbon is an amorphous carbon material which has excellent properties such as ultra-low friction, wear resistance, and chemical stability and then it is expected to be used in space stations, airplane engines, drones, medical equipment, etc. However, the wear of diamond-like carbon can lead to reduced material lifespan, machine failure, and even unexpected accidents. Therefore, minimizing its wear to the utmost is a critical challenge for realizing a safe and secure society. Especially, its wear behavior varies significantly even with slight environmental differences such as partial pressures of water vapor, oxygen, nitrogen, and hydrogen, and then experimental research has not yet advanced our understanding of its underlying mechanism. Therefore, it is strongly demanded to utilize computational science simulations for clarifying the effects of environments and atmosphere on its wear mechanism and then for establishing the design guidelines to reduce its wear. However, unlike “material-intrinsic properties” such as hardness and electrical conductivity, the changes in wear phenomena due to the environments represent “material response characteristics”. Therefore, understanding multi-physics phenomena including chemical reactions, friction, impact, stress, fluids, and heat transfer by computational science simulations is essential, which is one of the challenging tasks in computational science simulations.

Therefore, by developing a reactive molecular dynamics simulator capable of elucidating complex multi-physics phenomena involving chemical reactions on the supercomputer “MASAMUNE-IMR,” for the first time in the world we discovered that wear occurs via two mechanisms, chemical wear and mechanical wear, on diamond-like carbon and revealed that the chemical reactions occurring on the surface of diamond-like carbon during friction vary depending on the environments such as water and oxygen, leading to differences in the form and amount of chemical wear and mechanical wear. This achievement contributes to extending the lifespan of mechanical systems as well as preventing failures and accidents.

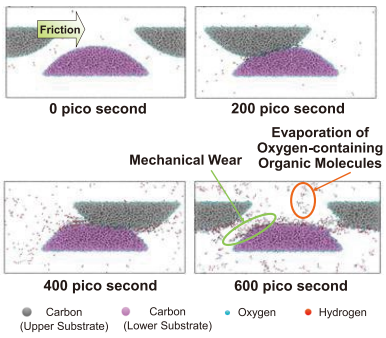


Figure. Friction simulation of diamond-like carbon under water environment (Water hidden for clarity).
We have demonstrated that water molecules dissociate into H^+ and OH^- at carbon atoms with dangling bonds on diamond-like carbon surfaces, initiating chemical wear where oxygen-containing organic molecules such as methanol and ethanol evaporate.

Jing Zhang, Yang Wang, Qian Chen, Yixin Su, Shandan Bai, Yusuke Ootani, Nobuki Ozawa, Koshi Adachi and Momoji Kubo
Carbon, 231 (2025) 119713, DOI: https://doi.org/10.1016/j.carbon.2024.119713

02

High-T_c Superconductivity in an Effective Hamiltonian for Bilayer Nickelates

High-temperature (high-T_c) superconductivity has recently been reported in the bilayer nickelate $La_3Ni_2O_7$ under high pressure. In this study, we focused on the bilayer Hubbard model as a minimal model for its relevant electronic states. The model describes electrons moving on two coupled square-lattice layers with strong repulsion between electrons occupying the same site. Despite its simple form, accurately solving the model is challenging because of strong electron correlations.

We performed large-scale numerical calculations on a supercomputer using cluster dynamical mean-field theory, which accurately treats dynamical electron correlations. The calculations revealed high-T_c superconductivity and showed that strong correlations play an essential role in its emergence.

The metallic state above T_c also exhibits unusual behavior. As shown in the lower panel of Figure, correlation effects become more pronounced from right to left, and part of the low-energy electronic spectral weight is strongly suppressed in the strongly correlated regime. This pseudogap behavior is also a characteristic feature of high-T_c cuprate superconductors, suggesting that nickelates and cuprates may share common physics originating from strong electron correlations.

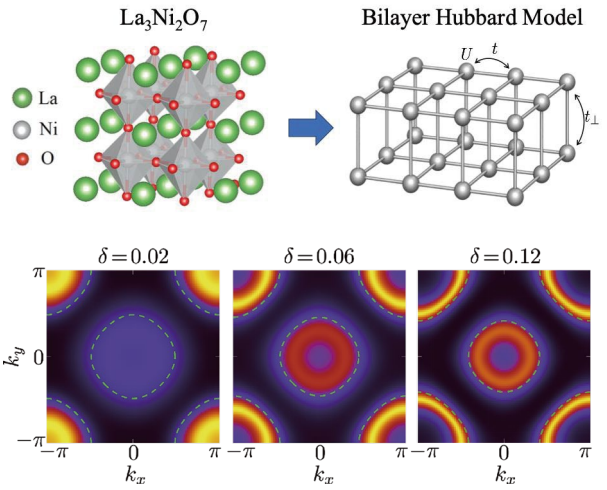


Figure. Bilayer Hubbard model for $La_3Ni_2O_7$ and its electronic states. The upper panel shows the model derived from the crystal structure, while the lower panel shows the momentum distribution of low-energy electronic states. In the strongly correlated regime (left), a pseudogap appears.

Yusuke Nomura, Motoharu Kitatani, Shiro Sakai and Ryotaro Arita
Phys. Rev. B, 112 (2025) L020504, DOI: https://doi.org/10.1103/dygc-94fq

03

Balancing Reactivity and Ion Transport in Mg Alloy Anodes via Secondary-Phase Engineering

Solid-state Mg metal batteries are promising for safe and high-energy storage, yet their performance is limited by unstable anode/electrolyte interfaces. The key challenge is to regulate, rather than eliminate, interfacial reactions: moderate reactions generate Mg^{2+} transport pathways, whereas excessive reactions cause passivation and polarization. This work shows that secondary-phase engineering can balance interfacial reactivity and transport in Mg alloy anodes. Density functional theory calculations establish a descriptor-guided framework for alloy/electrolyte interface design. Interface formation energies quantify the reaction tendency between Mg-alloy secondary phases and a $Mg(BH_4)_2$-based solid electrolyte, while charge density difference analysis reveals electron redistribution and bonding interactions. These calculations identify Mg_2Sn as a favorable secondary phase with controlled reactivity and reduced passivation risk. The resulting percolated Mg_2Sn network with continuous α-Mg pathways supports interfacial stability and Mg^{2+} transport. This work connects atomic-scale interface chemistry with alloy anode design and highlights controlled reactivity as a key principle for stable Mg alloy anodes.

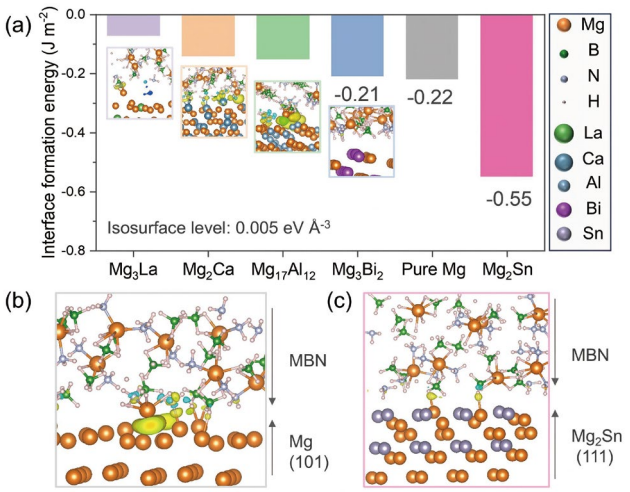


Figure. Reactivity and Mg^{2+} transport at Mg-alloy/solid-electrolyte interfaces regulated through secondary-phase engineering. (a) Interface formation energies of various Mg-alloy/MBN interfaces and atomic structures of (b) Mg(101)/MBN and (c) Mg_2Sn(111)/MBN interfaces.
MBN: $Mg(BH_4)_2{\cdot}2NH_3$.

Qian Wang, Xue Jia, Ting Xu, Jianwei Li, Yungui Chen, Hao Li and Yigang Yan
ACS Energy Lett., 11 (2026) pp.4621-4628, DOI: https://doi.org/10.1021/acsenergylett.6c00909

04

Lattice Oxygen Insertion Mechanism in Cerium Oxide Catalysts

Cerium oxide (CeO_2) is an important catalyst widely used in organic synthesis as well as environmental and energy-related applications. However, the molecular-level origin of its high catalytic activity has remained largely unclear. In this study, we employed first-principles molecular dynamics simulations in conjunction with enhanced sampling techniques to investigate the nitrile hydration reaction in aqueous solution. We discovered a previously unknown reaction mechanism in which a surface lattice oxygen atom, rather than an oxygen atom originating from the solvent water, is incorporated directly into the product. This theoretical prediction was further verified experimentally using oxygen isotope labeling. The direct participation of lattice oxygen has generally been considered to occur only in high-temperature reactions, but our study provides the evidence that lattice oxygen can actively participate in catalytic reactions even under mild conditions near room temperature.

The free energy calculations required extensive first-principles molecular dynamics simulations, which were enabled by the massively parallel computing environment of MASAMUNE-IMR. This computational platform made it possible to elucidate complex solid–liquid interfacial reactions at the atomic level. The findings of this study not only advance our understanding of the reaction mechanism of CeO_2 catalysts but also provide valuable insights into the rational design of high-performance catalysts.

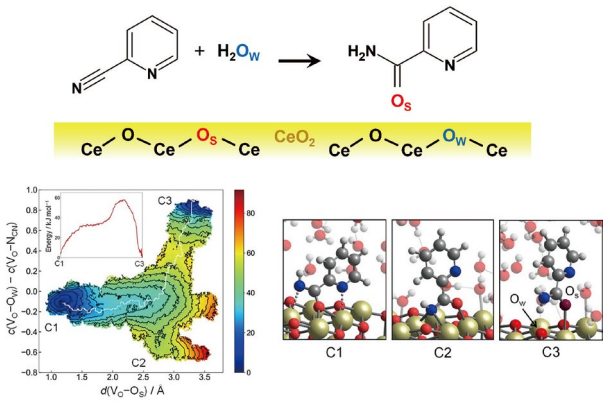
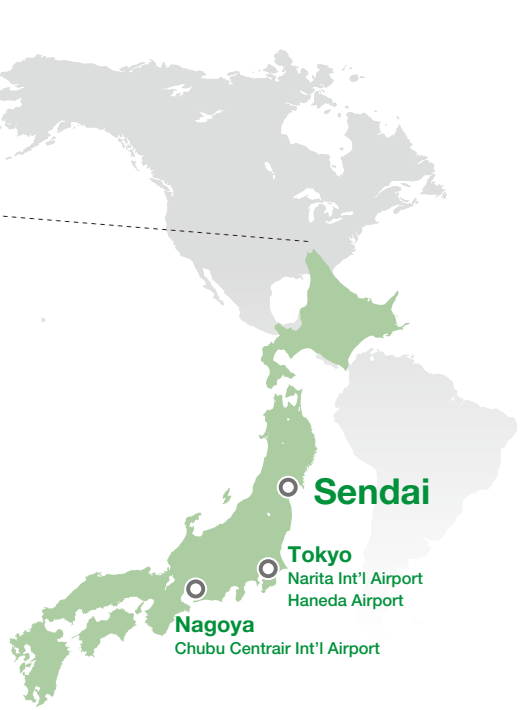


Figure. Free energy analysis of the nitrile hydration reaction over a CeO_2 catalyst. First-principles molecular dynamics simulations revealed that the reaction pathway involving incorporation of a surface lattice oxygen atom into the product proceeds with a lower free energy barrier than the conventional pathway involving an oxygen atom derived from water.

Takaaki Endo, Tatsushi Ikeda, Koki Muraoka, Yusuke Kita, Masazumi Tamura and Akira Nakayama
Chem. Sci., 16 (2025) pp.939-951, DOI: https://doi.org/10.1039/d4sc06294a

Access



Haneda Airport (Tokyo/Haneda)
- Tokyo Monorail / Keikyu Line
- 15 min
- Hamamatsucho Station / Shinagawa Station
- JR Yamanote Line
- 15 min

Narita International Airport (Tokyo/Narita)
- Narita Express
- 1 hour

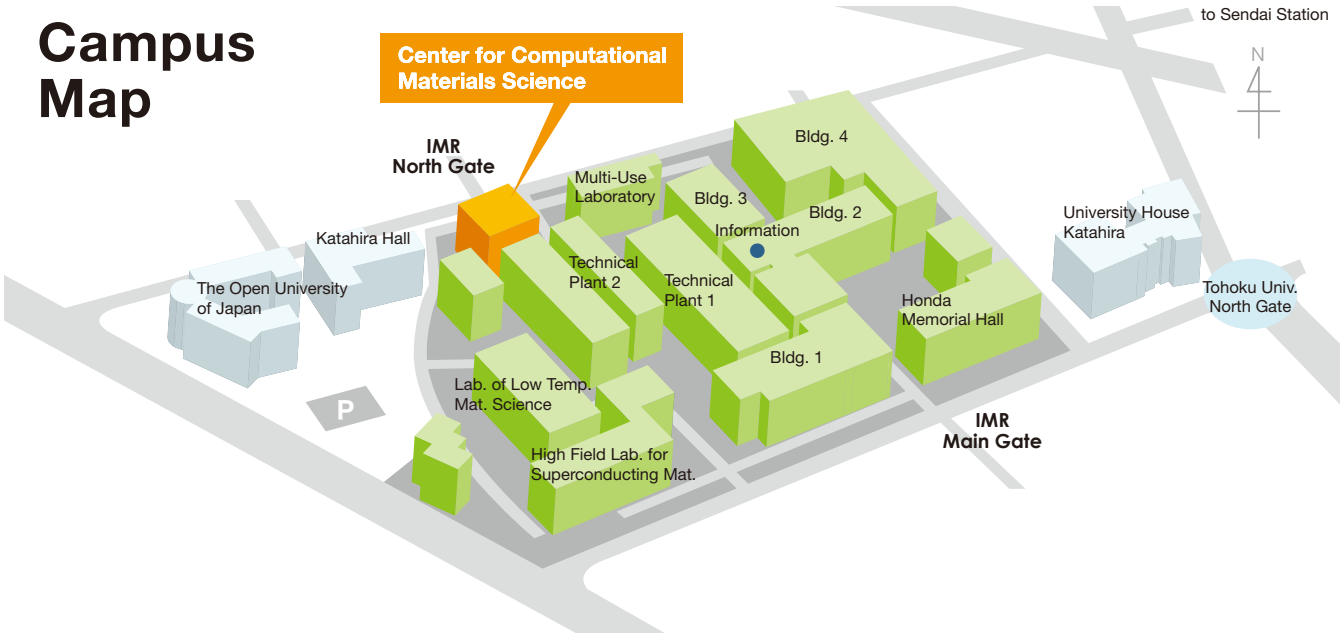
Chubu Centrair International Airport (Nagoya)
- Airplane
- 1 hour 30 min
- Sendai Airport
- Sendai Airport Access Line
- 25 min

JR Tokyo Station
- Tohoku Shinkansen
- 1 hour 30 min

JR Sendai Station
- A Taxi Stand (1F)
- 10 min

Institute for Materials Research, Tohoku University

Campus Map





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