CCMS

Center for Computational Materials Science
Institute for Materials Research
Tohoku University

MASAMUNE-IMR

MAterials science Supercomputing system for Advanced MUlti-scale simulations towards NExt-generation - Institute for Materials Research

TOHOKU UNIVERSITY

Supercomputing System

Greeting

Head, Momoji KUBO

Great expectations towards the computational materials science have been growing and growing in recent years in order to create prosperous and livable future society. Especially, for solving many problems facing humanity, such as addressing energy and environmental issues as well as establishing safe, secure, and sustainable society, computational materials science is expected to play key and crucial roles. Flagship supercomputer Fugaku in Japan won the first place in TOP500, world computer performance ranking, in June, 2020. Furthermore, Fugaku won the first place in HPCG (High Performance Conjugate Gradient), HPL-AI, and Graph500. Under these circumstances, our supercomputer in Center for Computational Materials Science (CCMS) belongs to the second level in the domestic computational resource hierarchy where Fugaku supercomputer is in the first level and is strongly required to contribute to the development and advancement of materials science. In order to fulfil our mission above, CCMS provides computational resources to materials science community as an international collaborative research institute as well as promotes the development of application software for supercomputer and its application to materials science. CCMS also provides computational resources to the researchers who participate in the projects of Program for Promoting Research on the Supercomputer Fugaku, Professional development Consortium for Computational Materials Scientists (PCoMS), and Element Strategy Initiative as a project of Supercomputer Consortium for Computational Materials Science. Furthermore, CCMS cooperates with the PCoMS project, assists the parallelization of application software, and holds the lecture courses for application software. In addition, CCMS established Computational Materials Science Forum (CMSF) in May, 2020, with 1) Center of Computational Materials Science, The Institute for Solid State Physics, The University of Tokyo, 2) Institute for Molecular Science/Research Center for Computational Science, National Institutes of Natural Sciences, and 3) Institute for NanoScience Design, Osaka University. CMSF performs activities to gather opinions about the indispensable and requisite future simulation technologies and future data utilization technologies, and to make their recommendations to the national government and its related organizations.

Since August 2018, CCMS has started the operation of supercomputing system “MASAMUNE-IMR”, which has Cray XC50-LC and Cray CS-Storm 500GT as main supercomputers. Total operation performance of this system is 3 PFLOPS, which is 10 times faster than our previous supercomputing system of 300 TFLOPS. CCMS aims to clarify and confront the mission of CCMS in the materials science field, to promote the cooperation and integration with different research fields, and to advance the creative and innovative researches, 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 consists of 1) supercomputer Cray XC50-LC, 2) supercomputer Cray CS-Storm 500GT with GPU accelerator, 3) and other servers, in order to satisfy diverse research needs in computational materials science field. The total theoretical peak performance of the two main supercomputers is 3 PFLOPS. This system is specialized for materials science simulations, having various application software for materials design tuned for our supercomputer, and is provided to the domestic and foreign researchers of the materials science field.

Mission of Center for Computational Materials Science

Supercomputing system of Center for Computational Materials Science (CCMS) has been used by the researchers of materials science field as a collaborative research institute in Institute for Materials Research (IMR) through renovating the supercomputing systems several times since the first introduction of the supercomputing system in 1994. CCMS established frameworks as a domestic collaborative research institute in 2009 and has contributed to producing a wide variety of creative and innovative achievements in materials science field by providing the computational resources to materials science researchers. Furthermore, in 2018 CCMS was certified as an international collaborative research institute.

The system renovation in 2018 makes it possible to provide new computational resources which satisfy diverse research needs such as GPU-based massively parallel computing, multi-scale simulations, and materials informatics, in addition to the conventional demands such as prediction of physical phenomena and materials design. This renovation aims at contributing 1) to the innovation of materials research technologies for solving energy and environmental problems, 2) to the development of device/electronics materials for creating prosperous and livable future society and for strengthening Japan's international competitiveness, and 3) to developing new social infrastructure materials for realizing safe, secure, and sustainable society. CCMS also hopes to contribute to the advancement and promotion of computational materials science field and community in the world by releasing the leading-edge results obtained by the maximum utilization of our supercomputing system.

Furthermore, CCMS provides the computational resources to the researchers who participate in the projects of Program for Promoting Research on the Supercomputer Fugaku, Professional development Consortium for Computational Materials Scientists (PCoMS), and Element Strategy Initiative as a project of Supercomputer Consortium for Computational Materials Science. Furthermore, CCMS also cooperates with the PCoMS project, assists the parallelization of application software, and holds the lecture courses for application software, in order to provide active supports for the advancement and promotion of computational materials science field and community in the world.

MASAMUNE-IMR

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Supercomputing System Configuration Diagram

Total Theoretical Peak Performance of Supercomputer: 3.03 PELOPS

System integrated by Hitachi, Ltd.

1 Supercomputer (Large-Scale Parallel Computing Server)

Cray XC50-LC

- Total Nodes: 320 nodes
  - Computing Node: 293 nodes
  - I/O Node, etc .: 27 nodes
- Total Theoretical Peak Performance: 0.91 PFLOPS
- Total Memory Size: 219.8 TiB

2 Supercomputer (Accelerator Server)

Cray CS-Storm 500GT

- Total Nodes: 29 nodes
- Total Theoretical Peak Performance: 2.12 PFLOPS
  - CPU: 0.09 PFLOPS
  - GPU: 2.03 PFLOPS
- Total Memory Size: 21.8 TiB

3 Storage System

DDN EXAScaler ES14KX

- Total Disk Capacity: 4.0 PB

DDN GRIDScaler SFA7700X

- Total Disk Capacity: 435.0 TB

4 Parallel Computing & Informatics Server

HPE ProLiant DL360 Gen10

- Total Nodes: 29 nodes
- Total Theoretical Peak Performance: 0.10 PFLOPS
- Total Memory Size: 16.3 TiB

5 Visualization Server

HPE ProLiant DL380 Gen10

6 Network System

HPE ProLiant DL360 Gen10

Nickname and Front Panel Design of Supercomputing System

MASAMUNE-IMR

MAterials science **S**upercomputing system for **A**dvanced **MU**lti-scale simulations towards **NE**xt-generation - **I**nstitute for **M**aterials **R**esearch

Nickname “MASAMUNE-IMR” is given to the supercomputing system of CCMS. This nickname is from “Masamune Date” who was the first lord of Sendai in the 17th century and dispatched the sailing ship “San Juan Bautista” in 1613 towards the world from Sendai. “Masamune Date” is drew on the front panel of our supercomputer by Sumi-E Artist OKAZU, with the letters “MASAMUNE-IMR” . This “Masamune Date” on the front panel is looking ahead to the next-generation materials science of the world from Sendai. In the nickname, “MASAMUNE-IMR” , we express our hope that creative and innovative achievements of the advanced multi-scale simulations on materials science obtained by our supercomputing system will give great impacts towards the next-generation from Sendai to the world.

■ “MASAMUNE-IMR” is a registered trademark of Tohoku University.

Proposal of Non-Empirical Atom-by-Atom Wear Law for Precision Micromechanical Systems

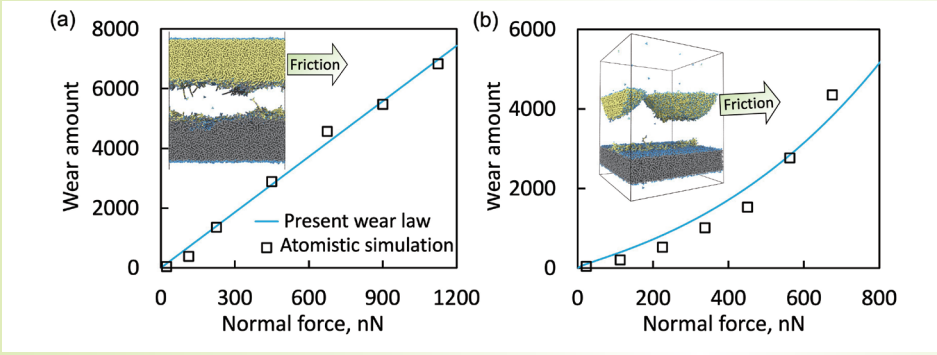


Fig. Wear amounts of diamond-like carbon obtained by wear law and atomistic molecular dynamics simulation.
- Wear amounts of (a) rough-surfaces and (b) ball-on-disk contacts show different dependence of loads. These figures prove that the very simple wear amount prediction law constructed in this study is able to quantitatively predict the wear amount obtained by long-time molecular dynamics calculations using the supercomputer.

In recent years, precision micromechanical systems used in drones, robots, automobiles, medical instruments, etc., have been developing at an accelerating rate, in response to the growing demands for them. However, when micromechanical systems are driven in a drone, robot, automobile, medical instrument, etc., the materials of the micromechanical systems rub against each other causing wear, which seriously damages their accuracy and durability. Especially, because micromechanical systems are extremely small in size, even a very small amount of wear, which is not a problem in normal size mechanical systems such as engines, motors, transmissions, etc., causes great damages to the entire systems. Therefore, it is strongly required to reduce the amount of wear to the utmost limit.

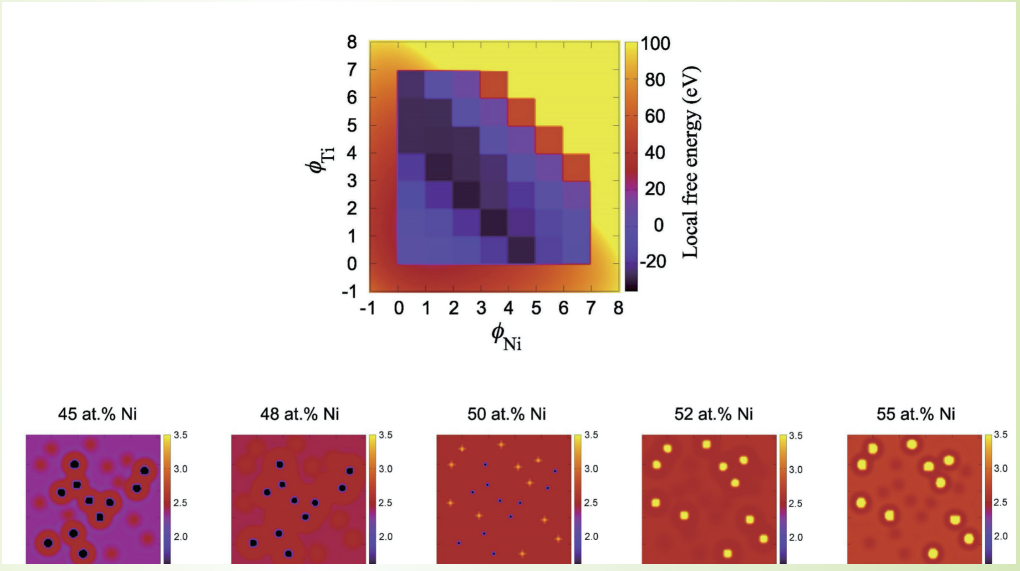
To prolong the life of mechanical systems and to improve their durability by solving the above problem, it is necessary to establish a theoretical law that can quantitatively predict how much wear will occur depending on the materials and usage conditions before conducting experimental research. However, in micromechanical systems, this wear phenomena occur at friction interfaces of tens of nanometers. Therefore, unlike visible wear which occurs in normal size mechanical systems such as engines, motors, and transmissions, nano-scale wear which cannot be seen by the naked eyes and is dominated by atomistic chemical reactions is the main factor in the micromechanical systems. Therefore, it has long been pointed out that the conventional wear prediction law for normal size mechanical systems cannot be applied to micromechanical systems, however this problem has not been solved for a long time.

Therefore, by developing a reactive molecular dynamics simulator that can elucidate complicated multi-physics phenomena including chemical reactions on the supercomputer “MASAMUNE-IMR”, chemical reaction mechanisms which induce wear at the friction interface of micromechanical systems are clarified. By applying the reaction rate theory to the above chemical reaction mechanisms, we proposed a non-empirical atom-by-atom wear law for predicting the wear amounts of materials for micromechanical systems. Furthermore, we simulated the wear amount of diamond-like carbon by reactive molecular dynamics method using the supercomputer and then proved that the very simple wear amount prediction law constructed in this study is able to quantitatively predict the wear amount obtained by long-time molecular dynamics calculations using the supercomputer. This result contributes not only to prolonging the life of micromechanical systems but also to the prevention of breakdowns and accidents.

Yang Wang, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Koshi Adachi, and Momoji Kubo
Adv. Sci., 8 (2021) Art.No.2002827, https://doi.org/10.1002/advs.202002827

Microstructures of Ni-Ti alloys using the first-principles phase field method

The upper panel shows the 2D map of the local free energy of Ni-Ti alloys where at most two interstitial atoms are considered in the tetrahedron approximation. The values for the compositions Ni_nTi_m with $n+m\leq 6$ are determined by first-principles calculations. The Ni concentration, ϕ_{Ni}, and the Ti concentration, ϕ_{Ti}, are discretized as $n\leq\phi_{Ni}<n+1$ and $m\leq\phi_{Ti}<m+1$, and each square box corresponds to one (n,m).
The lower panel shows he steady spatial distributions of the Ni concentration, ϕ_{Ni}, calculated by the first-principles phase field method only using the local free energy shown in the upper panel without any empirical parameter for Ti-45at%Ni, Ti-48at%Ni, Ti-50at%Ni, Ti-52at%Ni, and Ti-55at%Ni. The resulting patterns are almost the same as those without considering interstitial atoms, though some of the cuboidal or angular precipitations are rotated, and orange crosses appear around the yellow spots for Ti-50at%Ni. This rotation is reasonable, because no rotation along with the simulation cell axes is an artifact when we did not consider the interstitial atoms. The interstitial configurations do not appear in the final microstructure although they could influence the dynamics.

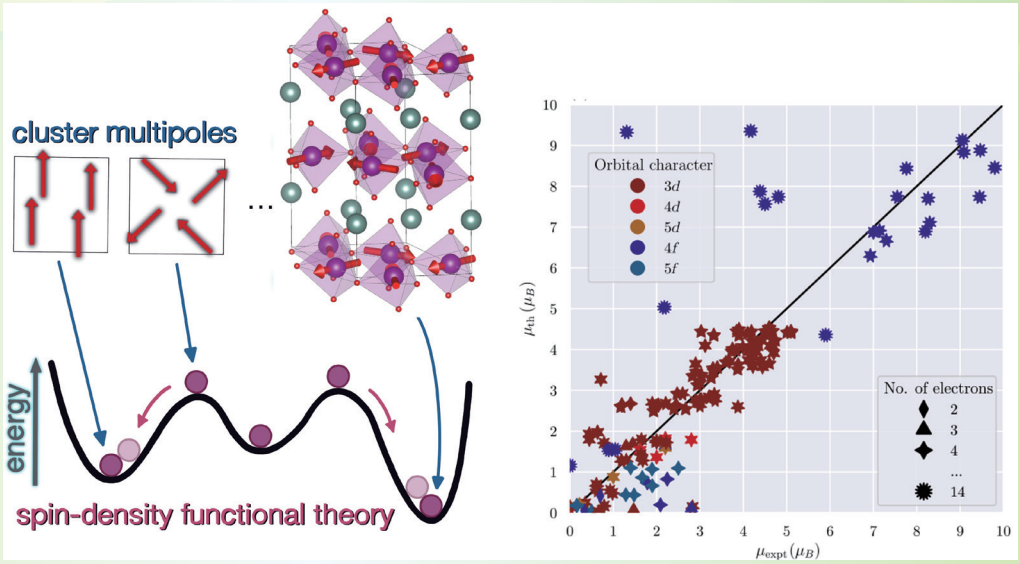


Kaoru Ohno, Monami Tsuchiya, Riichi Kuwahara, Ryoji Sahara, Swastibrata Bhattacharyya, and Thi Nu Pham
Comp. Mat. Sci., 191 (2021) Art.No.110284, DOI:https://doi.org/10.1016/j.commatsci.2021.110284

Simulation Results by IMR Supercomputing System

Ab Initio Prediction of Magnetic Structures Based on Cluster-Multipole Theory

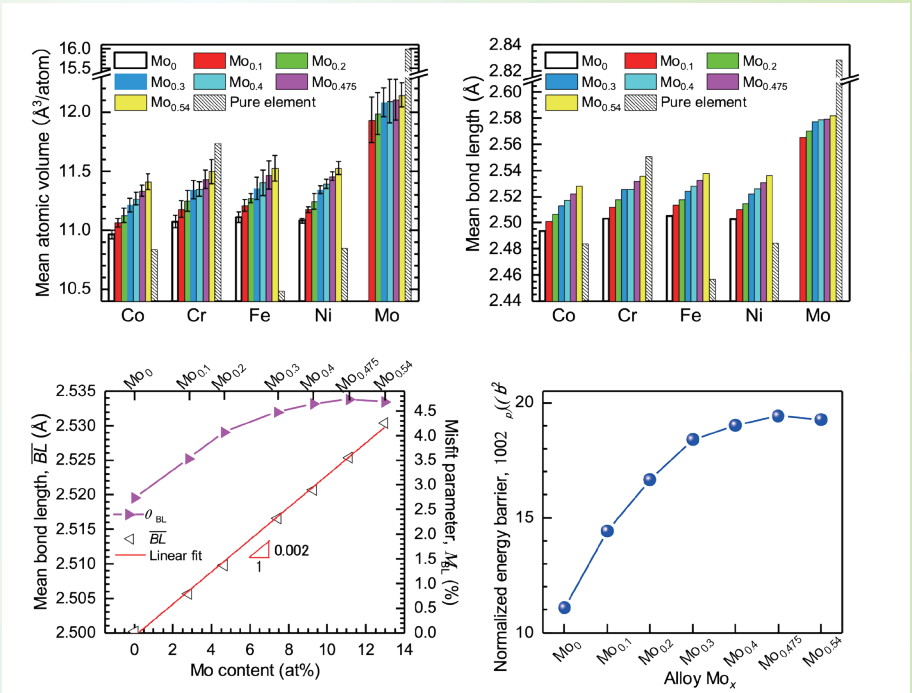
In a magnetic material, magnetic moments align themselves with their neighbors in very specific formations. While the magnetic structure determines the physical properties of magnets, accurate prediction of the spin configuration is one of the grand challenges in solid state physics. This is due to the presence of many degrees of freedom in the system. In this study, we device the cluster multipole (CMP) theory to treat the degrees of freedom in a physically meaningful way, and create an exhaustive list of candidate magnetic structures for which we performed a high-throughput calculation with ~3,000 possible magnetic structures. With the combination of the CMP theory and the local spin-density approximation (LSDA) for noncollinear magnetism, our study lays a solid foundation for the *ab initio* predictions of various magnetic properties by showing that (1) the CMP expansion administers an exhaustive list of candidate magnetic structures, (2) CMP+LSDA can narrow down the possible magnetic configurations to a handful of computed configurations, and (3) LSDA reproduces the experimental magnetic configurations with an accuracy of ~0.5 μB.



M.-T. Huebsch, T. Nomoto, M.-T. Suzuki, and R. Arita
Phys. Rev. X, 11 (2021) Art.No.011031, DOI:https://doi.org/10.1103/PhysRevX.11.011031

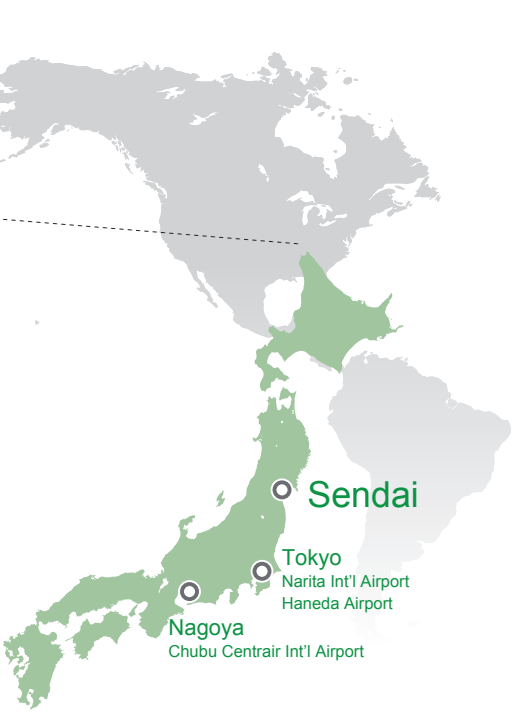
Solid-solution strengthening enhanced by Mo addition into NiCoCrFe-based high-entropy alloys

By *ab initio* simulations, the degree of lattice distortion for Mo-added NiCoCrFe-based high-entropy alloys (HEAs) was precisely evaluated. The atomic volumes and bond lengths (BL) of the constituent elements in the off-equiatomic Mo_x HEAs (x = 0, 0.1, 0.2, 0.3, 0.4, 0.475, and 0.54) ascended with increasing the Mo content. However, the increase in the mean BL ($\overline{BL}$) was not significant (0.2% per at%Mo), indicating that the effect of lattice expansion on the solid-solution strengthening was minimal. In contrast, the misfit parameter σ_{BL}, which corresponds to the standard deviation of BL, increased significantly at first, changed slowly after the $Mo_{0.3}$ HEA, and peaked at the $Mo_{0.475}$ ($Ni_{1.8}Co_{0.95}Cr_{0.8}Fe_{0.25}Mo_{0.475}$) HEA. This indicates that Mo atoms induce large lattice distortion locally in the NiCoCrFe-based solid-solution HEAs. The most severe lattice distortion in the $Mo_{0.475}$ HEA resulted in the highest energy barrier for the dislocation glide. The experiment validated the highest yield stress in the homogenized $Mo_{0.475}$ HEA.



J. Li, K. Yamanaka, and A. Chiba
Mater. Sci. Eng. A, 817 (2021) Art.No.141359, DOI:https://doi.org/10.1016/j.msea.2021.141359

Access



Haneda Airport (Tokyo/Haneda)
- Tokyo Monorail → 15 min → Hamamatsucho Station
- Keikyu Line → 15 min → Shinagawa Station
- JR Yamanote Line → 15 min → JR Tokyo Station
- Tohoku Shinkansen → 1 hour 30 min → JR Sendai Station

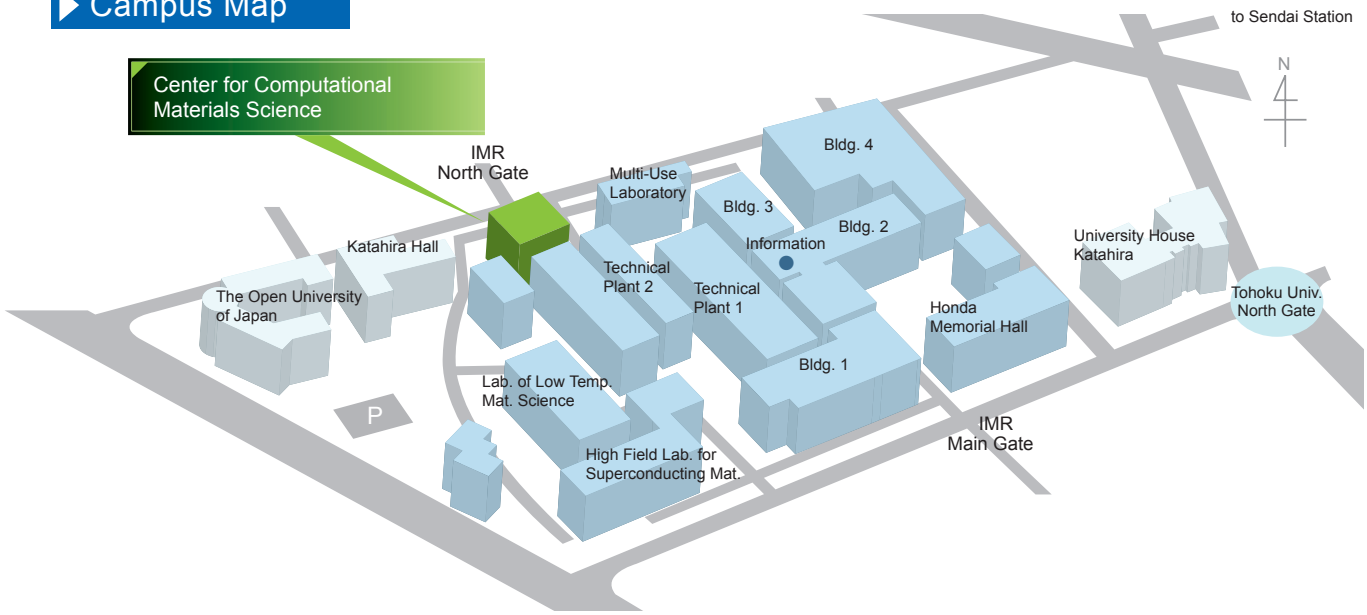
Narita International Airport (Tokyo/Narita)
- Narita Express → 1 hour → JR Tokyo Station
- Airplane → 1 hour → Sendai Airport
- Sendai Airport Access Line → 25 min → JR Sendai Station

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

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

Institute for Materials Research, Tohoku University

Campus Map



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