

## **3.5 SCCMS Projects**

# Development of molecular simulation framework for studying mesoscale liquid dynamics

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I now work on a large-scale molecular simulation of the dynamics of liquids. This year was in the phase of developing new code. The achievements are described in two parts in the following, in which simulations on the scale of millions of atoms (particles) are enabled.

## 1 Development for large-scale electrolyte simulators

Dilute electrolytes, water with a small amount of dissolved ions, are indispensable for functional properties in, for example, biological function and batteries. For the purpose of elucidating many-body properties produced by correlated ions, million-atom scale molecular dynamics simulations may provide valuable insights by directly incorporating the cooperative effects induced by electrostatics.

In this year, I have developed molecular simulation code for TIP4P/2005 water + ions, based on Framework for Developing Particle Simulator (FDPS) [1], FDPS provides a library that automatically produces spatial decomposition by the recursive multi-section method associated with tree construction for fast communication between different MPI processes, which means that the users can concentrate on implementing force fields and time development schemes. Importantly, tree method ensures scaling with  $O(N \log N)$ , bypassing the necessity for using FFT that prevents parallel scalability. Currently, I have achieved the speed of 12,000 steps per day for a system with 192,000 atoms. Further application tuning is ongoing, targeting 50,000 steps per day

on ISSP System B (Ohtaka).

## 2 Development simulators for long-time correlations in glasses

When a liquid is rapidly cooled down, it turns into a glass with solidity, keeping the random atomic configurations. About two years ago, I have revealed power-law correlations in the long-time behavior of the velocity autocorrelation function in such a supercooled liquid in two dimensions. In order to fully address such a long-time correlations both in two and three dimensions, it is necessary to calculate time-dependent trajectories of each individual particle. This brings about difficulties in MPI parallelization using the spatial decomposition, because particles are no longer bound to the memory of a specific CPU. In FY2020, I have added some time-series analysis code for shared memory environment to my existing distributed parallel code for a Lennard-Jones binary mixture with Kob-Andersen parameters. The whole codes are also extended to equip CUDA routines, enabling us to calculate the autocorrelations on shared memory environment by accelerating the force-field calculation on GPUs. I am currently using this for studying space and time correlations in 2D and 3D glass-forming liquids with  $O(10^7)$  particles.

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## Creating a Wannier function database toward material design

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As a numerical scheme for non-empirical analysis of electronic states in strongly correlated materials, the development of a calculation method based on first-principles calculations has been actively studied in recent years. In this method, the effective Hamiltonian describing the low-energy degrees of freedom is derived from the band structure obtained by the first-principles calculation [1]. The derived *ab-initio* effective Hamiltonian can be analyzed with high accuracy using low-energy solvers such as numerical exact diagonalization [2] and multivariate variational Monte Carlo methods [3] to reveal the electronic states of real solids in a non-empirical manner. On the other hand, these analyses require a high level of expertise and experience in the generation of the Wannier function, which is required in the derivation of the effective Hamiltonian. If this task can be automated, it will be possible to automatically generate model analyses for various materials, which will greatly expand the framework of material design.

In this project, we have developed a tool for automatic generation of Wannier functions and made dataset for machine learning. The Wannier functions can be calculated using the first-principles calculation software Quantum

ESPRESSO (QE) [4] and Wannier90 [5]. In order to create a dataset, we have modified a tool *cif2qewan* [6] made by T. Koretsune group at Tohoku Univ. to output the input files for QE calculation from *cif* files containing crystal structures. By downloading *cif* files from the Materials Project [7] under certain conditions and using them with this tool, we performed comprehensive calculations of Wannier functions and created a dataset.

First, we performed exhaustive calculations for about 1000 substances as a trial calculation. As a result, the calculation was successful for about 400 materials, and about 10 Wannier functions were generated for each material. In order to increase the efficiency of data generation, it was found that it could be reduced to about 10% by controlling the parameter values. We also found that the bottleneck area, which takes a lot of computation time in Wannier90, could be speeded up by MPI parallelization, and we succeeded in achieving a 10-times speedup after making changes.

In future research, we plan to perform high-throughput calculations using the tools created and accelerated in this project to create datasets of Wannier functions, and also to try to automatically generate Wannier functions using

machine learning such as deep learning. This research was done by collaboration with T. Koretsune, K. Kurita, and T. Oikawa of Tohoku Univ., T. Misawa of Beijing Academy of Quantum Information Sciences, K. Ido of Institute for Solid State Physics, and TOYOTA MORTOR CORPORATION.

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- [6] <https://github.com/wannier-utils-dev/cif2qewan>
- [7] <https://materialsproject.org>

# Computational Investigation of Charge Photogeneration in Organic Solar Cells by Fragment-Based GW/BSE Method

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Accurate calculations of electronic states are essential for computational studies of organic materials which are directed toward understanding of fundamental processes in organic electronic devices. We have recently developed the large-scale GW method based on the fragment molecular orbital method. The fragmentation approximation for the total polarization function and the  $\Delta$ COHSEX approximation have been employed for efficient evaluations of GW quasiparticle energies from localized molecular orbitals. More recently, we have proposed the novel large-scale excited-state methods based on the FMO, exciton model, and GW/BSE with Tamm-Dancoff approximation (TDA). In this method, the excited-state Hamiltonian matrix elements at the GW/TDA-BSE level is calculated in the basis of fragment configuration state functions which describe intrafragment excitations or interfragment charge-transfer excitations. The excited-state Hamiltonian is then diagonalized to approximate the adiabatic excited states of an entire system. We have confirmed that for molecular clusters, the novel fragment-based GW/TDA-BSE can reasonably reproduce the excited states obtained from conventional GW/TDA-BSE method. Our developments enables the applications of GW/TDA-BSE method to large molecular assemblies, which will be useful for investigating charge separation in condensed phase.

As recent applications [1], we explore the

energy levels and charge-transfer states of the face-on and edge-on orientations of pentacene/C60 bilayer heterojunctions. FMO-GW/BSE calculations were performed for the local interface structures in the face-on and edge-on bilayer heterojunctions, which contain approximately 2000 atoms. Calculated energy levels and charge-transfer state absorption spectra are in reasonable agreements with those obtained from experimental measurements. We found that the dependence of the energy levels on interfacial morphology is predominantly determined by the electrostatic contribution of polarization energy, while the effects of induction contribution in the edge-on interface are similar to those in the face-on. Moreover, the delocalized charge-transfer states contribute to the main absorption peak in the edge-on interface, while the face-on interface features relatively localized charge-transfer states in the main absorption peak. Our results indicate that optimizing the molecular orientation and interfacial morphologies is essential for improving the power conversion efficiency of organic solar cells.

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# Promising Cathode Materials for Sodium-ion Rechargeable Batteries: *Ab initio* investigations

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We have studied two types of promising cathode materials applicable for sodium-ion rechargeable batteries.

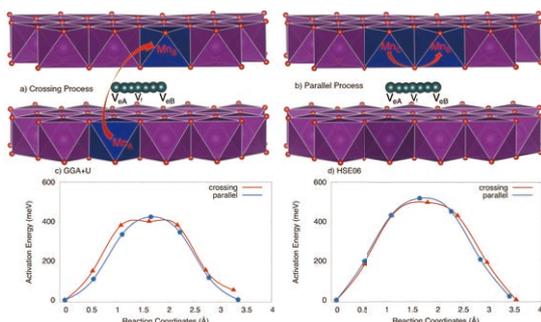


Fig. 1: Elementary diffusion processes at full charging states, including (a) crossing process and (b) parallel process and activation energy profile of Na vacancy–positive polaron complex obtained by (c) GGA+ $U$  and (d) HSE06 methods. The dark blue octahedrons represent the 3NN Mn sites where polaron formed, and the dark cyan balls stand for Na vacancy trace diffusion. The other Na atoms are hidden for more clarification.<sup>[1]</sup>

## 1. Na<sub>x</sub>MnO<sub>2</sub> layered oxide

P2 layered oxide Na<sub>x</sub>MnO<sub>2</sub> exhibit a voltage window from 2.0 to 3.5V and high specific capacity up to 220 mAh/g. However,

the material suffers from the serious phase transformation during its charging/discharging. Using the first principles density functional theory, we explored systematically its geometric, electronic properties, phase stability and diffusion mechanism for Na<sup>+</sup> migration. It is found that at high or low Na concentration, Na<sup>+</sup> ions prefer locating only at the edge-shared prism, while at  $x=0.5$ , the material become more stable with the ratio of the Na ion at edge-shared Na<sub>e</sub> and face-shared Na<sub>f</sub> prism of Na<sub>e</sub>:Na<sub>f</sub>  $\cong$  2:1. When all the Na<sup>+</sup> ions are deintercalated from NaMnO<sub>2</sub>, the conspicuous change in the lattice constant  $b$  causes an significant reduce of volume up to 20%. We pointed out that the hybridized orbitals of O's  $2p_y$  states and Mn's  $3d_{yz}$  and  $3d_{x^2-y^2}$  states, play an essential role in the electronic structure of the material. We proved the polaron formation and the polaron is preferably coupling with Na<sup>+</sup> vacancy/ion at the third nearest neighbor sites. Two elementary diffusion processes, including parallel and crossing processes, as shown in Fig. 1, could occur and require an activation energy of 423 meV (518 meV) at high Na

concentration and 273 meV (327 meV) at low Na content by GGA+*U* (HSE06) method. Compared to olivine phosphate, the Na<sup>+</sup> ion would diffuse better in Na<sub>x</sub>MnO<sub>2</sub> than in polyanionic framework like LiFePO<sub>4</sub> due to the significantly lower activation energy.<sup>[1]</sup>

## 2. Na<sub>x</sub>VPO<sub>4</sub>F

A new orthorhombic phase of tavorite-like Na<sub>x</sub>VPO<sub>4</sub>F cathodes ( $0 \leq x \leq 1$ ) applicable for Na-ion battery was proposed using density functional theory. We have explored the phase stability, electronic structures, electrochemical properties, and diffusion mechanisms of Na ions/vacancies of Na<sub>x</sub>VPO<sub>4</sub>F. No imaginary frequency in phonon dispersion provides evidence that the proposed material is thermally stable. It is suggested that the material can be synthesized from the reaction: NaF + VPO<sub>4</sub> → NaVPO<sub>4</sub>F because of the negative formation energy. The material NaVPO<sub>4</sub>F would undergo bi-phase reactions upon the Na deintercalation in the ranges of  $0.125 \leq x \leq 0.5$  and  $0.5 \leq x \leq 1$ , and show high voltages of 3.80 V and the high theoretical capacities of 143 mAhg<sup>-1</sup>. The polaron migration effect on the Na<sup>+</sup> ion diffusion mechanism was precisely investigated. Three elementary diffusion processes, including single, crossing and parallel processes, are indicated in Fig. 2. The parallel and crossing processes require much higher activation energy for Na<sup>+</sup> diffusion, implying a substantial polaron migration effect. The activation barriers of Na ion diffusion gain 323 and 530

meV in the Na-rich and poor contents, respectively. Therefore, the proposed cathode can be expected to exhibit significantly faster Na-ion diffusion than that in popular cathodes such as NaVOPO<sub>4</sub> (627 meV).<sup>[2]</sup>

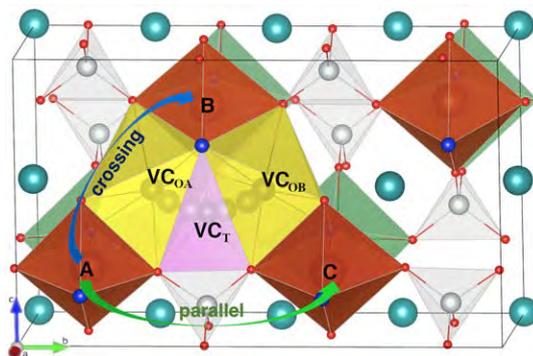


Fig. 2: Possible elementary diffusion processes of an Na vacancy (vc) accompanying by a positive polaron (pp) along the [010] direction in NaVPO<sub>4</sub>F. O (red), F (blue), V (brown), P (grey), Na (cyan), and vc (black) are shown by balls, and polyhedral structural units of V<sup>1NN</sup>O<sub>4</sub>F<sub>2</sub> (brown), V<sup>2NN</sup>O<sub>4</sub>F<sub>2</sub> (green), AO<sub>4</sub>F<sub>2</sub> (yellow) octahedra, and NaO<sub>3</sub>F (purple) tetrahedra are shown. When vc moves along a path from vco<sub>A</sub> to vco<sub>B</sub> via vct sites, pp can jointly hop from A to C sites (parallel process indicated by a green arrow), from A to B sites (crossing process indicated by a blue arrow), or remain at a same site (single process).

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# Ab initio study toward abundant element nanocatalysts with less precious metals

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DFT computations with QuantumEspresso (QE) are used to gain chemical insights and to design novel catalysts with abundant elements such as hexagonal boron-nitride (h-BN) for reducing costs and dependences on precious metals used in various heterogeneous catalysts.

We have shown that gold clusters supported on h-BN/Au(111) are highly active catalysts for hydrogen evolution reaction (HER) [1]. It is demonstrated that the most stable gold clusters on the h-BN/Au(111) support are not necessarily the most reactive; stabilization on the surface gold clusters with the different geometries and orientation with respect to the support can form a large variety of energetically favorable H adsorption sites considerably promoting HER activity. The charge transfer between the supported gold clusters and the h-BN/Au(111) surface promotes the catalytic activity of the Au<sub>n</sub>@h-BN/Au(111) system for HER. Therefore, h-BN/Au(111) can be considered as promising support for gold clusters as electrocatalysis [1].

Another application of BN is for oxidative dehydrogenation (ODH) of light alkanes such as olefin. Olefins are key feedstocks for range of commercially important chemicals such as polymers, fibers, and their derivatives, which are important for the energy and day to day applications. Therefore, a deeper insight into the mechanism and ways to explore catalysts for efficient oxidative dehydrogenation reaction is needed. We have proposed that oxygen functionalized h-BN with B-O-O-B sites

at the zigzag edges is active catalyst for ODH. This suggestion is consistent with experimentally reported concentration of B and N atoms (high B:N ratio) to explore the ODH mechanism in a series of light alkanes [2]. DFT calculations are performed to verify our proposal. We have explored the catalytic activity of the newly proposed oxygen functionalized edges of h-BN sheets for oxidative dehydrogenation of ethylbenzene. It is demonstrated that oxygen functionalized highly defective boron-nitride can demonstrate extraordinary catalytic activity for the above reaction [2].

We have elucidated the mechanism of the novel "heterocyclic segregation" reaction of one pyrazine ring with two nitrogen atoms into two quinoline rings with one nitrogen each. Our DFT calculations showed that the intramolecular ring-forming and -opening of nitrogen-heterocycles are strongly affected by the initial hydrogen-substrate interaction [3].

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# Development of high-performance permanent magnets by large-scale simulation and data-driven approach

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High-throughput first-principles calculation is a powerful tool for developing functional materials. However, systematic errors contained in computational data often prevent us from quantitative evaluation of physical properties. In order to overcome this problem, we have developed a data assimilation method in which a small number of experimental data are integrated with a large number of computational data [1]. Figure 1 is a schematic illustration of the method. Here, open circles denote accurate but a small number of data, whereas open squares are a large number of data that contain a systematic error. If we consider the former data only, we cannot estimate the target variable accurately for large  $x$  where the data do not exist, whereas accurate estimation is possible if we consider both the data. Based on this framework, we have developed a practical scheme for evaluating finite-temperature magnetization.

We have applied the scheme to  $(\text{Nd}_{1-\alpha-\beta-\gamma}\text{Pr}_\alpha\text{La}_\beta\text{Ce}_\gamma)_2(\text{Fe}_{1-\delta-\zeta}\text{Co}_\delta\text{Ni}_\zeta)_{14}\text{B}$  [1]. In the first step, we prepared 119 experimental samples, and measured the magnetization at 3-7 temperatures within a range from 300 K to 473 K. The magnetization at zero temperature ( $\mu_0M$ ) and Curie temperature ( $T_C$ ) are evaluated from these data by Kuzmin's formula. Independently, we performed systematic first-principles calculation for 2869 compositions using the KKR-CPA method. The saturation magnetization at zero temperature

is calculated in the local spin density approximation. The intersite exchange couplings are calculated using Liechtenstein's method, from which the Curie temperature is evaluated in the mean-field approximation. We then adopted the data assimilation, and obtained  $\mu_0M$  and  $T_C$  at arbitrary composition. The magnetization at arbitrary temperature is obtained using Kuzmin's formula. Figure 2 shows the magnetization at 0 K, 300 K and 400 K. We see that the magnetization monotonically decreases with increasing Co concentration ( $\delta$ ) at 0 K, whereas small amount of Co doping enhances the magnetization at 400 K.

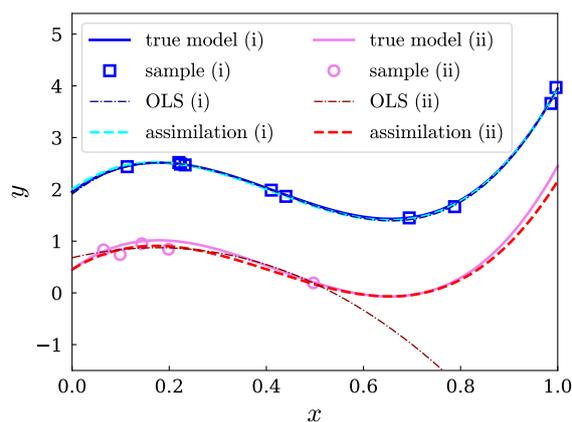


Figure 1: An example of the data assimilation.

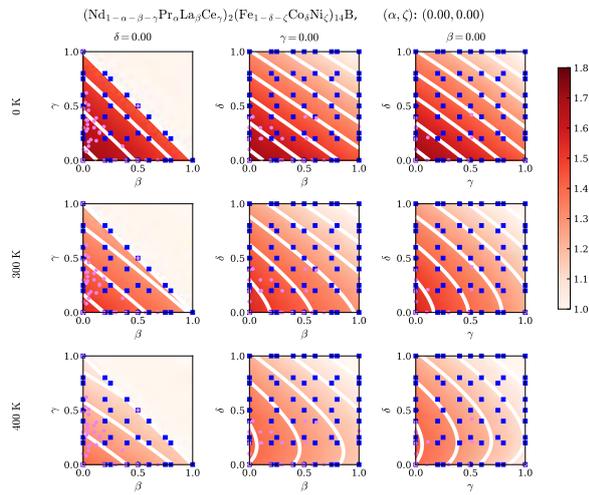


Figure 2: Magnetization of  $(\text{Nd}_{1-\beta-\gamma}\text{La}_\beta\text{Ce}_\gamma)_2(\text{Fe}_{1-\delta}\text{Co}_\delta)_{14}\text{B}$ .

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# Optimized design of magnetic materials based on the integration between quantum beam experiment and first-principles calculation

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We have been working on characterization and material design of rare-earth permanent magnets (REPMs) which is one of the most important materials for traction motors of vehicles and robotics. Quantification of REPMs has to be done on multiple length scales and energy scales, where our scope lies in the microscopic thermal equilibrium and off-equilibrium magnetization reversal process closer to the mesoscopic scales [1]. Since the main-phase ferromagnets in REPMs are typically made of multiple sublattices and each sublattice contributes to the bulk magnetic properties differently, it is an important problem to quantify the site-resolved contribution from the microscopic measurements to understand which sublattice can be more improved [2]. Based on the measured data from the neutron diffraction experiments, the Rietveld analysis can give us such information which so far has needed expertise of experienced practitioners. Still, unphysical solutions can be given as a metastable solution in the overall landscape of the cost function in the data fitting. In order to quickly select a physically meaningful solution and eliminate human bias as much as possible, we have been developing a data analysis technique combining Rietveld analysis and theoretical calculations [3, 4]. *Ab initio* electronic structure calculations for metallic ferromagnets can address site-specific magnetic moments based on the crystal structure data yielded by the Rietveld

analysis. The output of the *ab initio* calculation can be fed back into the Rietveld analysis and such hybrid process between measured data analysis and *ab initio* calculations can be iterated until the overall convergence is reached.

While the convergence in the hybrid analysis is quite fast in the ThMn<sub>12</sub>-type ferromagnets, feasibility for the Nd<sub>2</sub>Fe<sub>14</sub>B-type ferromagnets has been seen only recently with the new system B where the 128 cores can shorten the *ab initio* part based on AkaiKKR in less than an hour. This is in strong contrast to other electronic structure calculations for Nd<sub>2</sub>Fe<sub>14</sub>B which can take weeks on older machines. With the new hardware, the good *ab initio* calculation framework, and our new hybrid data analysis methodology, further developments of REPMs will be accelerated.

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# Evaluation of the polymer blend miscibility by using chain-increment method with all-atom molecular dynamics simulation

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Polymer blend, a mixture of polymers, may have distinct structural and dynamical features from the component polymers and is employed in a wide variety of applications including home appliances, biomedical devices, and automotive products. The mutual miscibility of polymer species is determined by the free energy of mixing. The mixing free energy is given by the changes in the (excess) chemical potentials between the pure and mixed states of the component species, and the chemical potentials reflect sensitively the effect of intra- and intermolecular interactions in turn. To approach the chemical potential of a polymer molecule, we formulated the method of chain increment and provided a scheme to compute the free energy of incrementing a monomer with all-atom models.[1] In this work, we extended the method and treated the single-component melts of polyethylene (PE), polyvinylidene difluoride (PVDF), poly(vinyl alcohol) (PVA), polyvinylpyrrolidone (PVP) in their linear forms.

## Results

The number of monomer units is fixed at 100 for all the systems. All-atom molecular dynamics simulation and free-energy

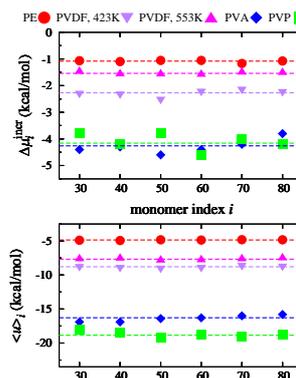


Fig 1: Incremental free energy  $\Delta\mu_i^{\text{incr}}$  and the average interaction energy  $\langle u \rangle_i$  against the index  $i$  of the incremented monomer in the tagged polymer at  $i = 30, 40, 50, 60, 70,$  and  $80$ . The horizontal, dashed line is the averaged value of  $\Delta\mu_i^{\text{incr}}$  or  $\langle u \rangle_i$ .

calculation has been conducted at 1 bar on the supercomputer system at ISSP. We compute the incremental free energy  $\Delta\mu_i^{\text{incr}}$  and the averaged interaction energy of the incremented monomer with the surroundings  $\langle u \rangle_i$ . Figure 1 shows that  $\mu_i^{\text{incr}}$  stays constant within a few tenths of kcal/mol for inner monomers, demonstrating the validity of the chain-increment method.  $\langle u \rangle_i$  is also constant against the index  $i$  of the incremented monomer, showing that the local environment around the monomer is independent of the monomer location along the polymer chain.

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# Development of high-throughput calculation tools and evaluation of magnetic properties in hard magnetic materials

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In this year, we developed (i) an automatic exhaustive calculation tool and (ii) an atomistic spin Monte Carlo simulation tool for permanent magnetic materials. Our automatic exhaustive calculation tool is based on the all-electron Korringa-Kohn-Rostoker (KKR) Green's function method (AkaiKKR code). The KKR Green's function method can be combined with the coherent potential approximation (CPA) which can treat configurational disordered systems, is quite useful for investigating the electronic structures, magnetic properties, and transport properties of rare-earth transition-metal alloys. In the CPA approach, the multiple scattering effect by disordered potentials is replaced with effective medium. Therefore, we can perform the electronic structure calculations for disordered materials without supercells and decrease the computation costs dramatically. Additionally, since a Green's function is directly obtained in the KKR method, we can efficiently investigate finite temperature magnetism and transport properties by the linear response theory. We applied this tool for and high entropy alloys and rare-earth magnet Sm-Fe-N systems and, succeeded in constructing large-scale magnetic material databases.

Atomistic spin Monte Carlo simulation was used for investigating the temperature dependent magnetization reversal in permanent magnets. The microscopic mechanism of the coercivity at finite temperature is a crucial

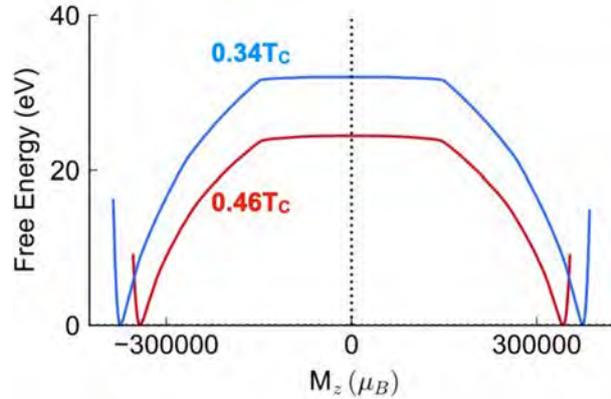


Figure 1: Free energy landscape for a isolated  $\text{Nd}_2\text{Fe}_{14}\text{B}$  particle by atomistic spin model simulation. The size of the particle is 14 nm, corresponding to 212,536 spins.

issue. Since the magnetization reversal is a stochastic transition from a metastable state to a stable state, we tried to capture the physical insight of the coercive force from the viewpoint of the free energy landscape. For the calculation of the free energy landscape, we developed a numerical simulation method for describing the magnetization reversal by nucleation, where highly efficient parallelization scheme (around 1,000–3,000 MPI parallelization) for the replica exchange Wang-Landau MC method and the reduction of systematic errors by the  $1/t$  method are implemented.

Applying the above method to the atomistic spin model with a isolated  $\text{Nd}_2\text{Fe}_{14}\text{B}$  particle, we performed the magnetization reversal anal-

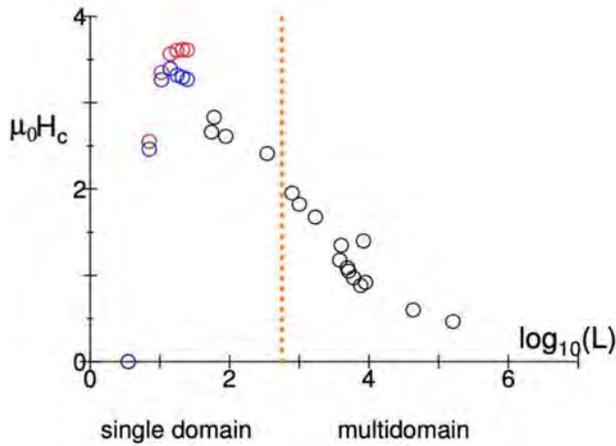


Figure 2: Coercive energy of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  at room temperature as a function of the size of the domain. The blue (red) circles indicate the calculation results without (with) the magnetic dipole interactions, respectively. White circles are the experimental results.

ysis for the effect of the thermal fluctuation and investigated the formation of the reverse nucleus which is a origin of the coercive force (see Fig. 1). It was considered that the barrier of the magnetization reversal is determined by the competition between the formation energy of the reverse nucleus and the Zeeman energy by external magnetic field: however, we newly proposed that the energy gain due to the expansion of the magnetization reversal region by the domain wall motion is a key role. This fact is quantitatively consistent with experimental results, where the size of the reverse nucleus dose not depend on external magnetic field.

In order to investigate the coercive force of permanent magnets quantitatively, we need to consider the effect of the magnetic dipole interactions (demagnetizing field). Although a convolution integral method (fast Fourier transform) is commonly used to incorporate long-ranged interaction, it is not effective for permanent magnet materials with low crystal symmetry such as  $\text{Nd}_2\text{Fe}_{14}\text{B}$ . We have developed a modified stochastic cutoff method that is applicable complex crystal structures with

long-ranged interaction in computational cost  $O(N\log N)$  without any approximations. This method can be combined with Monte Carlo simulation, leading to the quantitative analysis of the temperature dependent coercive forces of permanent magnets from the free energy landscape calculations with the magnetic dipole interactions (see Fig. 2). It is found that the influence of the magnetic dipole interaction (demagnetizing field) is strongly suppressed due to the surface thermal fluctuation.

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# Novel chloride solid electrolytes for all solid-state sodium metal battery

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Using high-throughput computing and structure database (Materials Project [1]), we evaluated exhaustively migration energies of Li, Na, and Mg ion in inorganic solids. Figure 1 presents the distribution of migration energies of Li, Na, and Mg ions in oxides by using BVFF-percolation approach.[2,3] The results indicate that various factors affect the ion conducting performance. Thus, materials informatics (MI) approaches are adopted to clarify the crucial factor for ionic conductivity in oxides. Among various regression approaches, gradient boosting regression shows the best prediction performance. However, the regression performance is not sufficient from the diagnostic plots shown in Fig.2. Our tentative analysis suggests that Li-O bond length and Li-O-Li bond angles are important, i.e. structural factors are more important than compositional factors. One of the reasons for rather poor regression performance may stem from low reproducibility of universal BVFF parameters.[2] To improve, high-throughput FF approaches[4] are used for 86 Na containing materials. In this technique, DFT-MD simulations are performed just for 2 ps, and then metaheuristically optimize FF parameters,

which is a derivative of original BVFF, to reproduce DFT-MD derived structural features, such as RDF and ADF. After that FF-MD approach is adopted to calculate the ion conductive performance. Figure 3 shows calculated Na ionic conductivities at room temperature for 86 compositions. We plan to verify reproducibility of present computation and apply MI approach for thus obtained data near future.

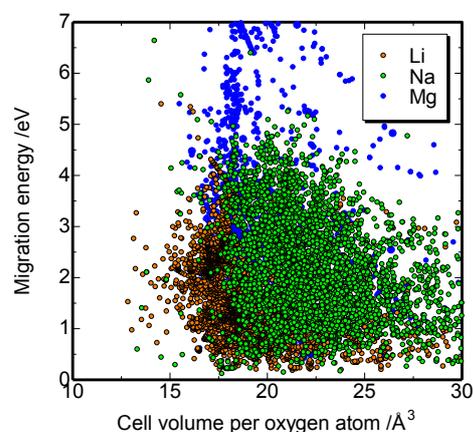


Fig. 1: Migration energies for Li, Na, and Mg ions (indicated by orange, blue, and green plots, respectively) calculated using automated exhaustive BVFF approach.

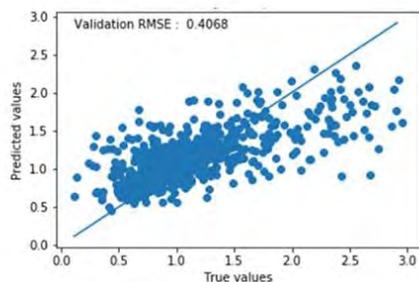


Fig. 2 diagnostic plot of the gradient boosting regression derived prediction function for Li migration energies in 711 Li-ion containing oxides.

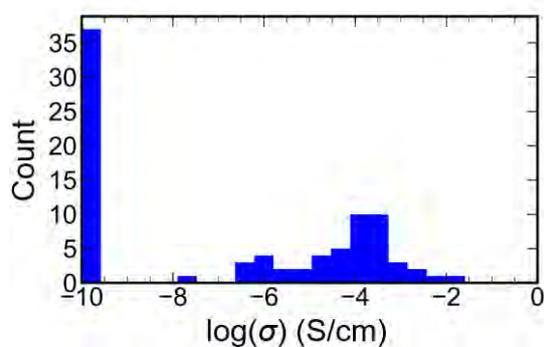


Figure 3 Histogram of room temperature Na ion conductivities for 86 samples using high-throughput FF-MD approach.

## References

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