JAMSTEC 国立研究開発法人 海洋研究開発機構
Japan Agency for Marine-Earth Science and Technology

Computational Performance of Quantum Mechanical Simulation on Earth Simulator

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- Coworkers -
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CSRN, School of Engineering Science, Osaka University, Japan

Outline

Quantum simulations = First-principles calculations
(not quantum computing)

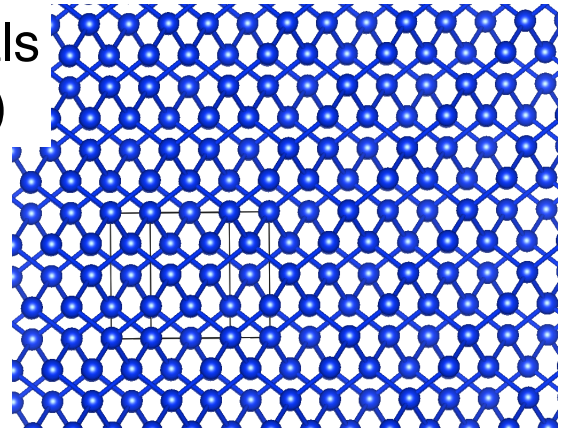
1. What is First-principles calculations
2. General Methodology of First-principles calculations
3. Applications
    1. using first-principles calculations (AkaiKKR)
    2. combining with model-based approaches.
4. Toward larger models; Earth Simulator GPUs
5. Summary

AkaiKKR is a quantum simulation package developed by our research group.
Earth Simulator is a high-performance computer managed by JAMSTEC.

What is First-principles calculations

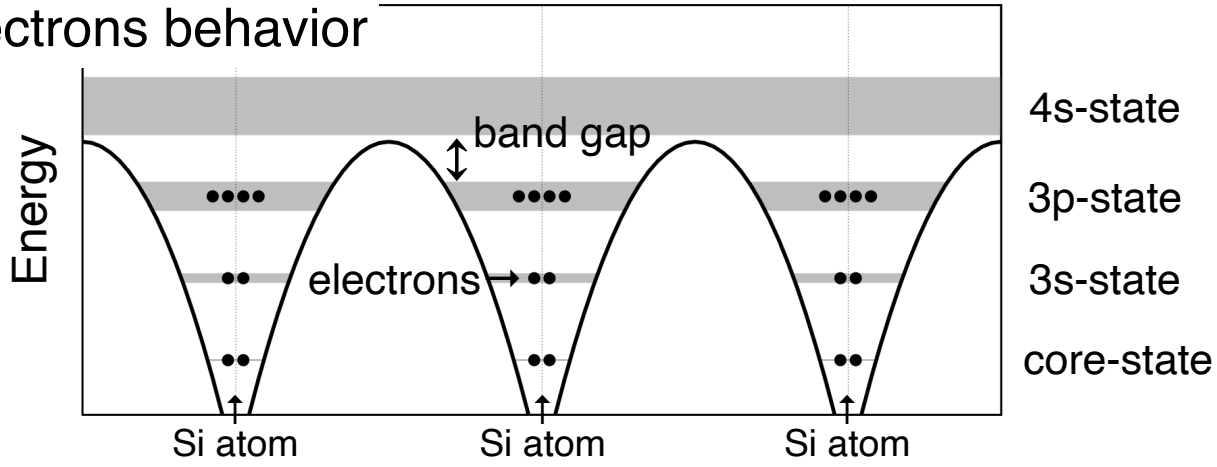
a method to speculate material properties from quantum mechanics

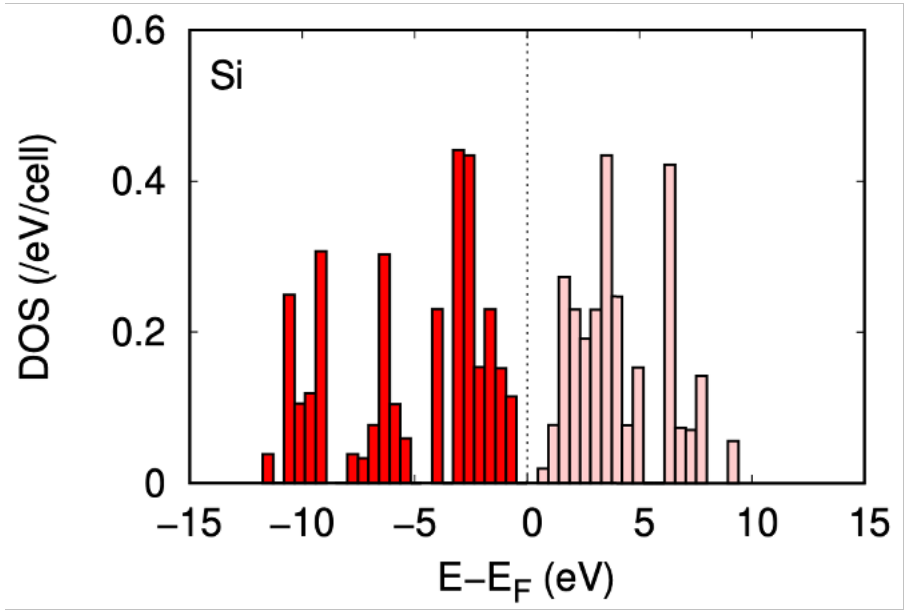
Si crystals (inputs)



simulations

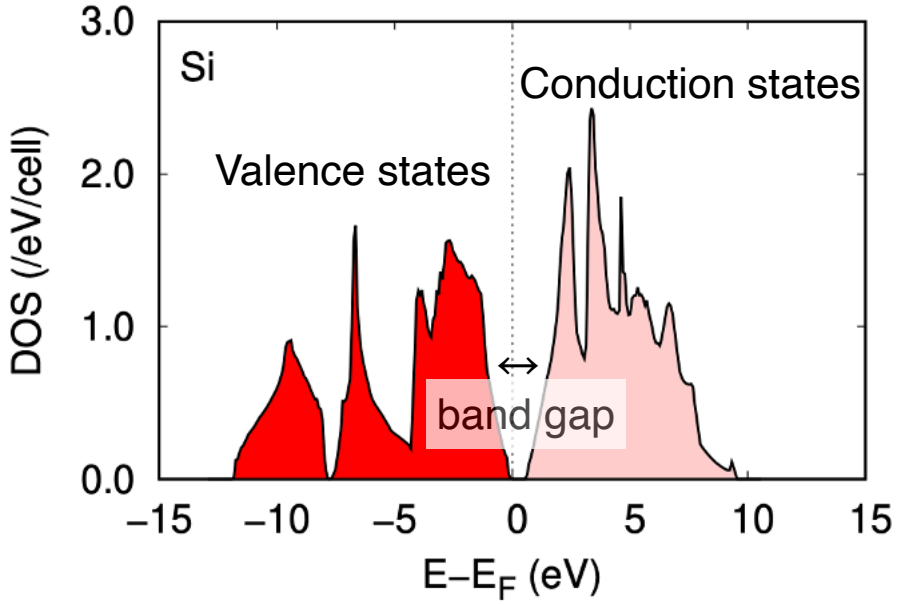
Electrons behavior





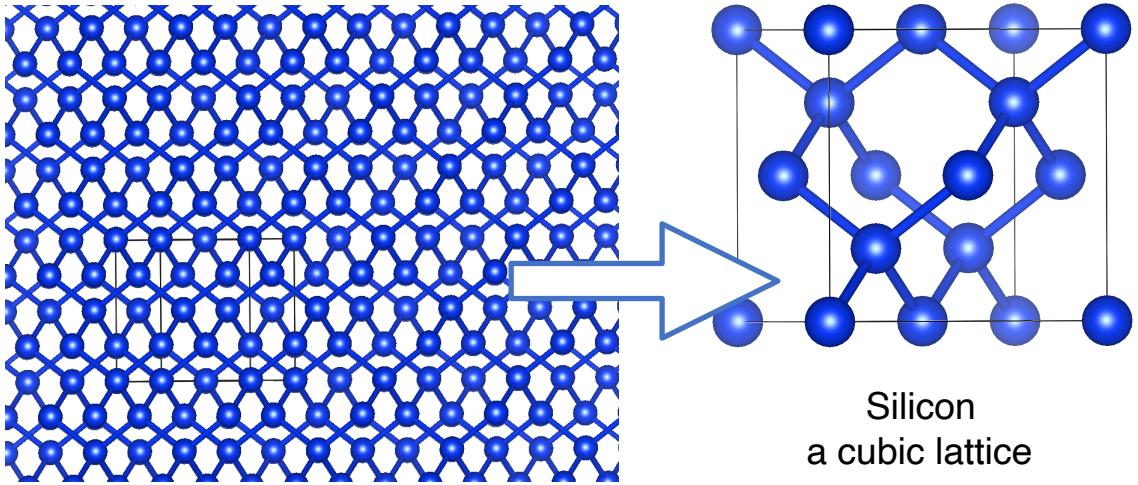
Density of States (DOS) = a simulation result

Increasing E-mesh



Simulations suggest Si crystals are insulating.

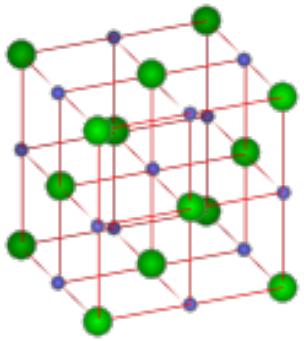
Model Structures in Quantum Calculations



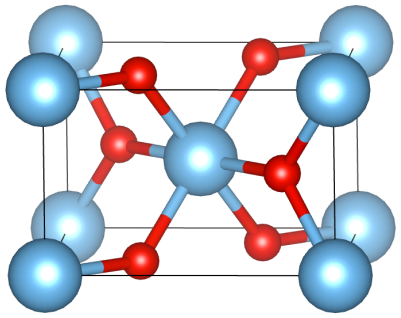
Silicon
a cubic lattice

Realistic crystal structures have too many atoms.
Approximation using a unit cell.
All crystals can be grouped to 7 species.

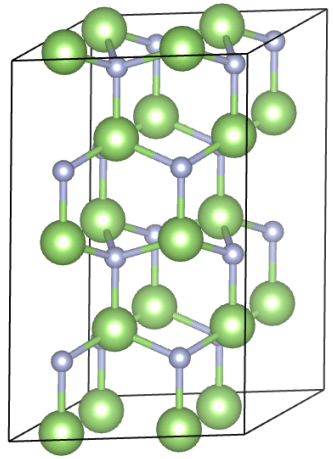
[1] view atomic structures by VESTA ©



NaCl
Rocksalt structure
a cubic lattice



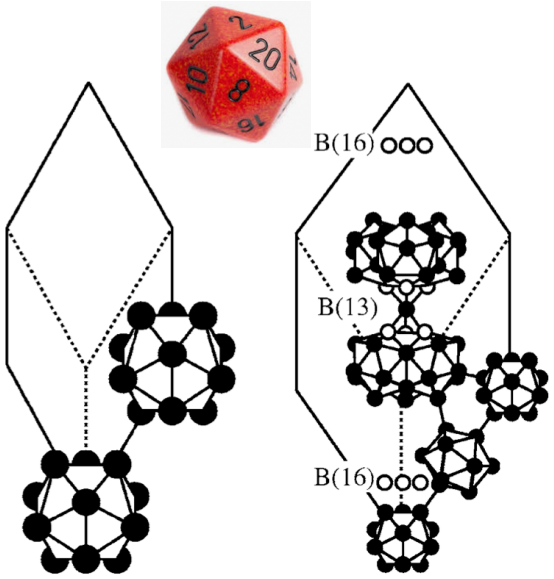
TiO2
Rutile structure
a tetragonal lattice



←
Gallium nitride
Wurtzite structure
a hexagonal lattice

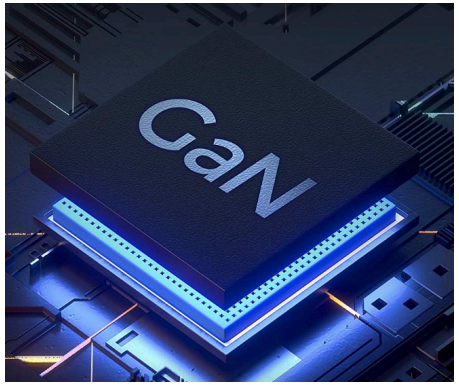
→
Solid boron
(α-phase、β-phase)

a rhombohedral lattice



Diluted Magnetic Semiconductors

CSRN, School of Engineering Science, Osaka University, Japan, studies *spintronics*.
(CSRN: Center for Spintronic Research Network)

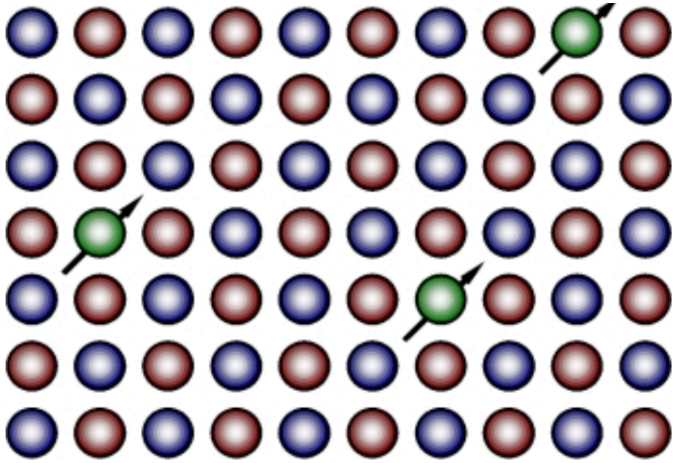


Semiconductors
(charge)

Magnets
(spin)

CPU, GPU

Spintronics = Spin Electronics



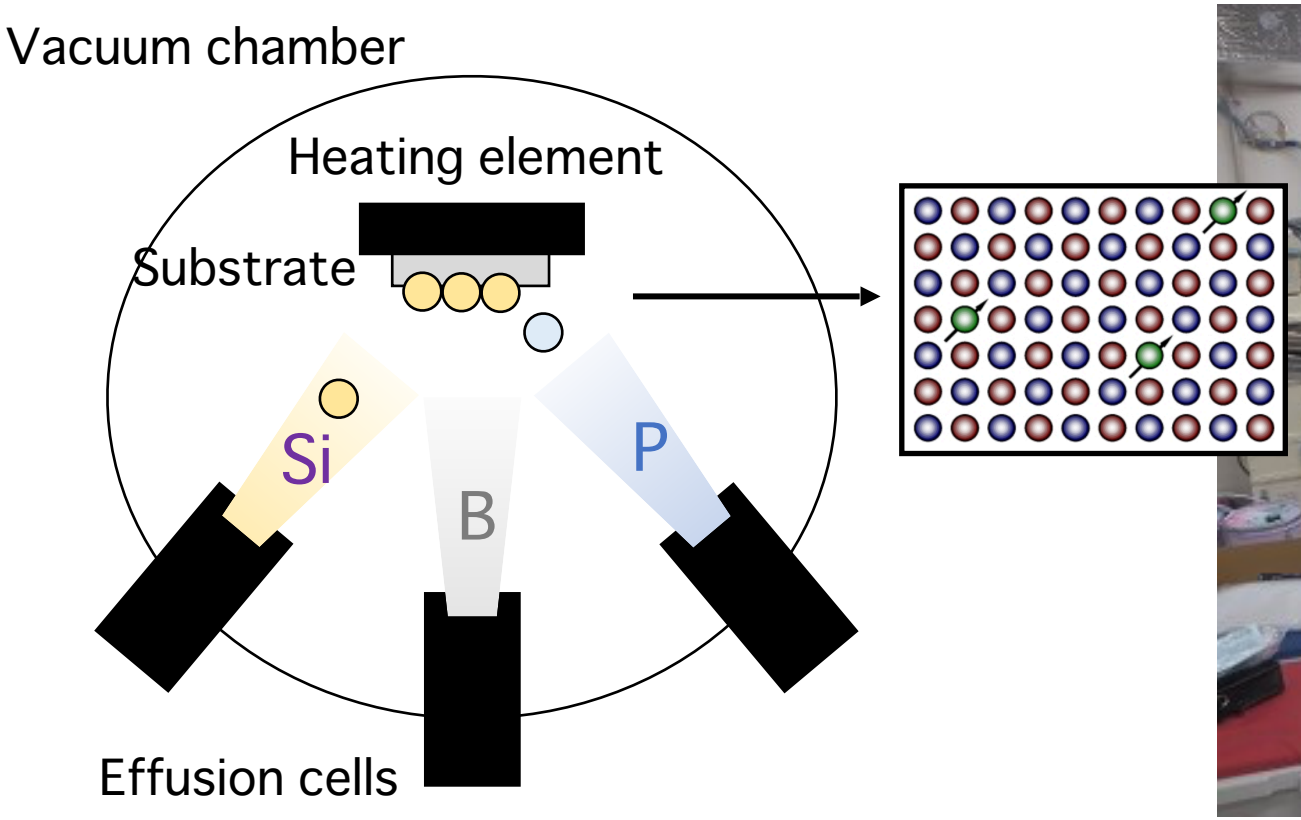
DAT, HDD

Study of
- spin of electron
- electron charge
- magnetic moment

e.g.)
- Diluted magnetic semiconductors
- Heusler alloys
- Quantum computing, neuromorphic

How to Make Semiconducting Materials

Molecular Beam Epitaxy (MBE)



A molecular beam epitaxy system
(Hamaya Group in Osaka Univ)

Property Evaluation by Simulation

The simulations are based on quantum mechanics

$$\mathcal{H}\psi = E\psi$$

First-principles calculations

Based on equation of motion for electrons
~ Microscopic standpoint ~

e.g. Schrödinger equation

$$\mathcal{H} = \sum_{i=1}^{N} \left\{ -\nabla^2 + v_{\mathrm{ext}}(\boldsymbol{r}_i) \right\} + \sum_{i \neq j}^{N} \frac{2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

- $-\nabla^2$: Kinetic energy
- v_{ext}: Atom potential
- 2nd term: Electron-electron interaction

This does not need empirical parameters.
This needs large computational costs

Model calculations

Constructed on the experimental results
~ Macroscopic standpoint ~

e.g. Heisenberg Model

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \boldsymbol{e}_i \boldsymbol{e}_j + \sum_i K(\boldsymbol{e}_i) + \mu B \sum_i e_i^z$$

- J_{ij}: Magnetic interaction
- $K(e_i)$: Anisotropic constant
- B: External magnetic field

These need empirical parameters.
These have reasonable computational costs.

Flow chart for first-principles simulation

load an atomic structure

initialize electron density

make Hamiltonian

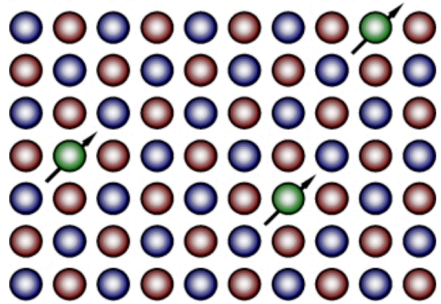
solve Hamiltonian

calculate new density

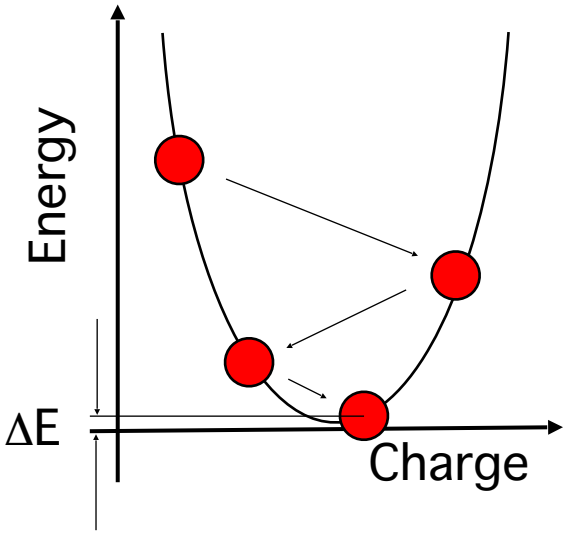
compare current and new density

get results!

Repeat
using new density



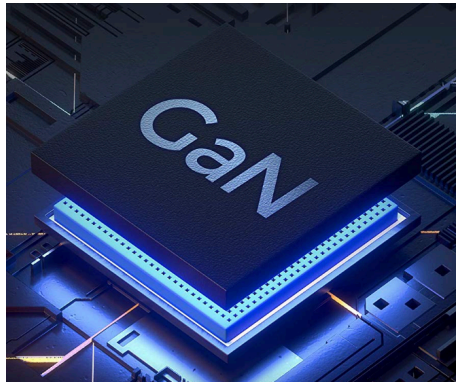
Self-consistent calculations

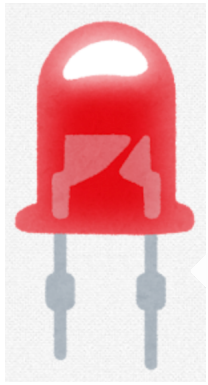


First-principles Calculations

e.g.) What happens by doping a rare earth (Eu) into GaN?

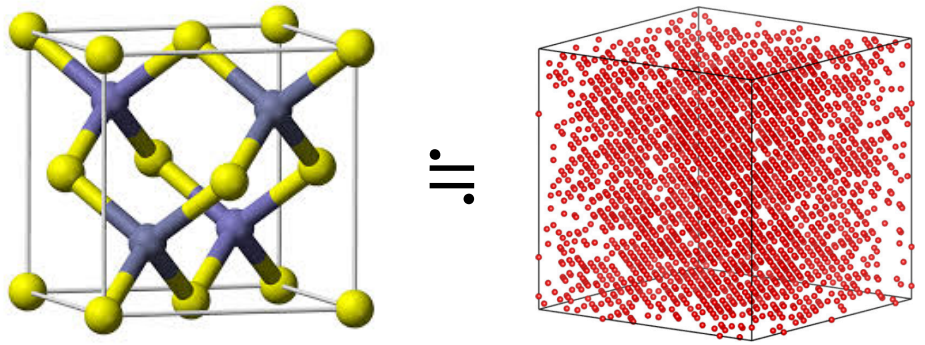
Eu-doped GaN: a diluted magnetic semiconductor





GaN is a next-generation semiconductor.
Rare earth elements; usage of LDE & magnets.

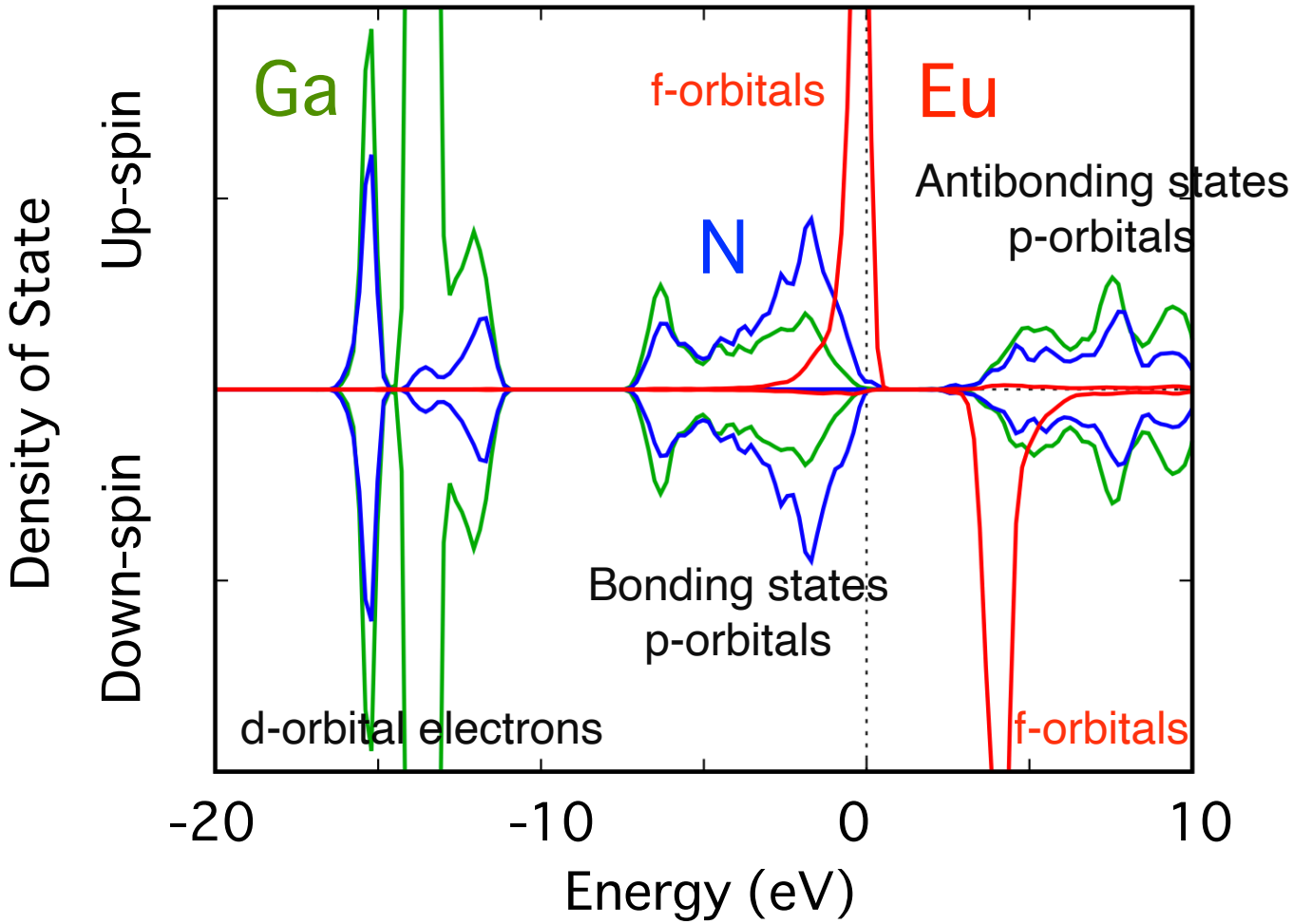
a Eu-doped GaN unit cell (left fig)
(Gray spheres: virtual atoms "Eu+Ga")



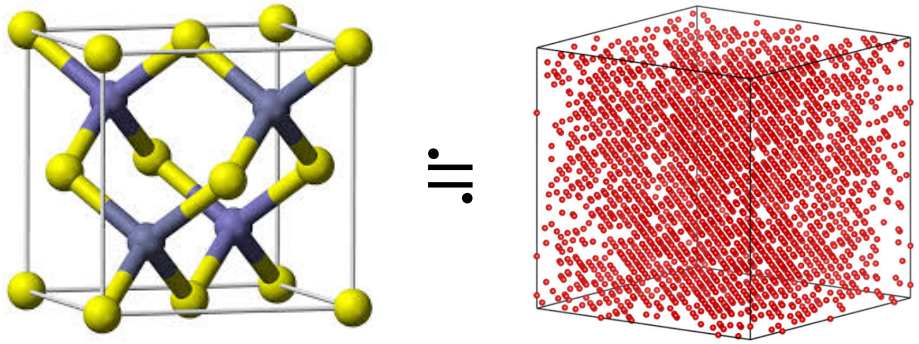
Eu was superimposed to Ga via CPA
to reduce the computational costs.
(CPA: an approximation of the mean field)
This model corresponds to a homogeneous
distribution of Eu atoms (right fig)

First-principles Calculations Results

1st evaluation: electronic structures



a Eu-doped GaN unit cell (left fig)
(Gray spheres: virtual atoms "Eu+Ga")



Eu was superimposed to Ga via CPA
to reduce the computational costs.
(CPA: an approximation of the mean field)
This model corresponds to a homogeneous
distribution of Eu atoms (right fig)

Simulation suggests ferromagnetism comes from f-orbital electrons in Eu.

First-principles Calculations Results

Another example: evaluation of phase separation

Free energy

$$E_{\mathrm{mix}} = \Delta E_{\mathrm{tot}} + k_{\mathrm{B}}T\left\{x\log(x) + (1-x)\log(1-x)\right\}$$

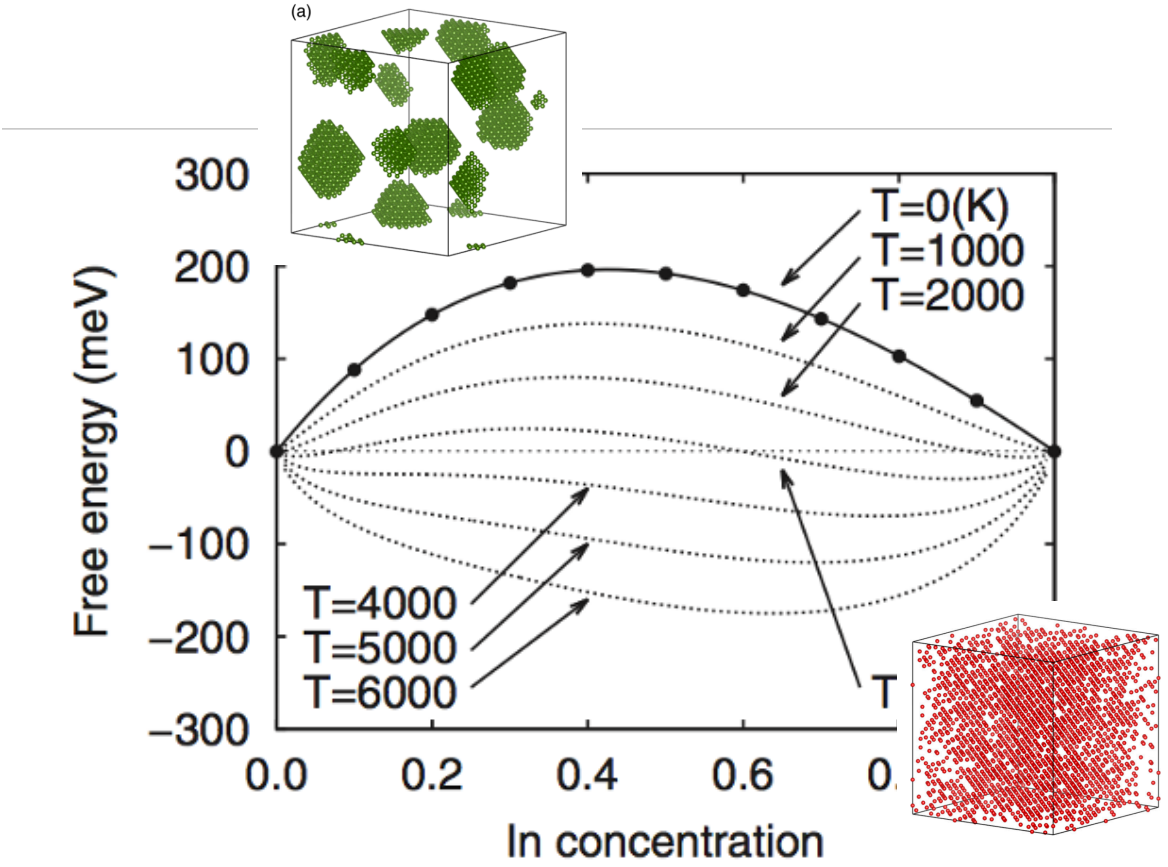
2nd term: Entropy term (x: concentration)

Total energy

$$\Delta E_{\mathrm{tot}} = E_{\mathrm{tot}}(\mathrm{Eu}_x\mathrm{Ga}_{1-x}\mathrm{N})$$

$$- xE_{\mathrm{tot}}(\mathrm{Eu}_x) - (1-x)E_{\mathrm{tot}}(\mathrm{Ga}_{1-x}\mathrm{N})$$

1st term: the doped system
2nd/3rd terms: non-doped systems



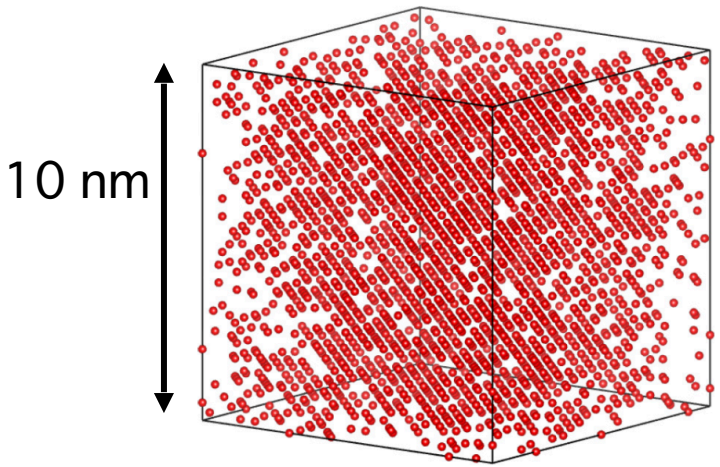
Simulation suggests phase separation occurs; nano-structures form in the crystal.
The models are so large that we cannot deal with them in first-principles calculations

A model calculation: simulation for crystal growth

Monte Carlo simulation was performed to generate Eu-doped GaN nano-structures.

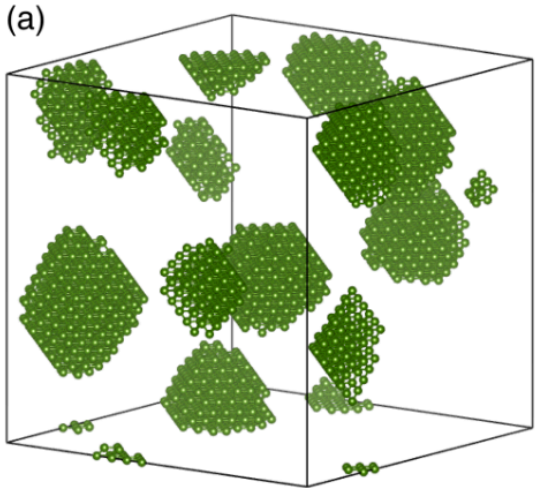
$$H = -\frac{1}{2}\sum_{i \neq j} V_{ij}\sigma_i\sigma_j$$

V_{ij}: Interatomic interaction of i and j

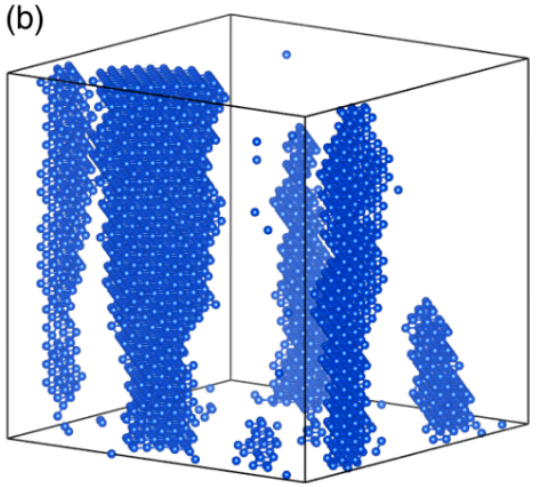


Eu Homogeneous distribution

32,000 atoms are included.



Eu quantum dots



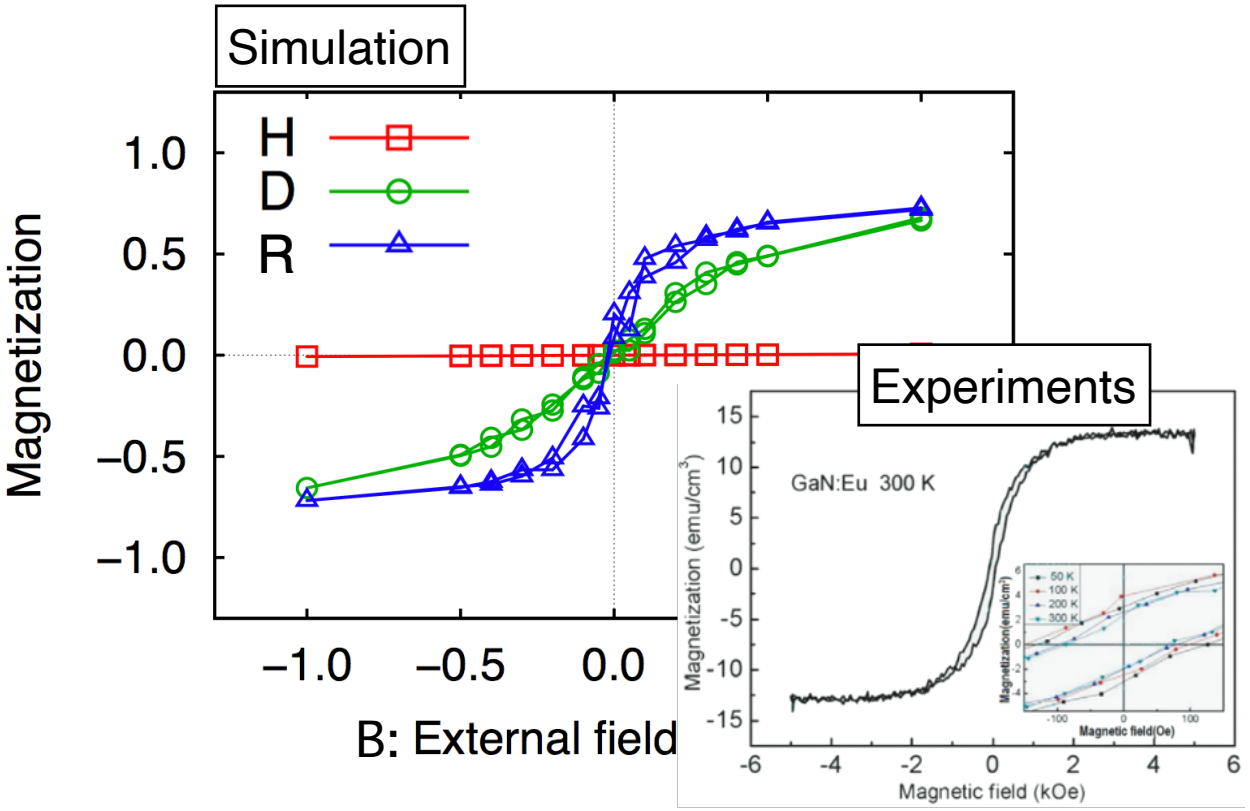
Eu quantum rods

[1] A. Masago, et al., Jpn. J. Appl. Phys. 55, 070302 (2016)

The models are so large that we cannot deal with them in First-principles calculations

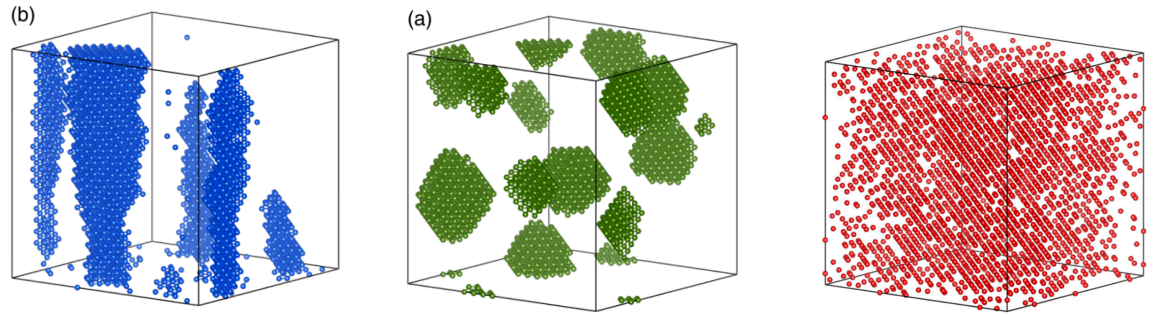
A model calculation: simulation for magnetization

Magnetization vs. External Field on Nano-structures



The Monte Carlo simulation was done with Heisenberg model:

$$\mathcal{H} = -\frac{1}{2}\sum_{i\neq j} J_{ij}\boldsymbol{e}_i\boldsymbol{e}_j + \sum_i K(\boldsymbol{e}_i) + \mu B \sum_i e_i^z$$



R: Quantum rods D: Quantum dots H: Homogeneous

[1] A. Masago, et al., Phys. Rev. B 98, 214426 (2018)

If we insist on using first-principles calculations, what other options do we have?

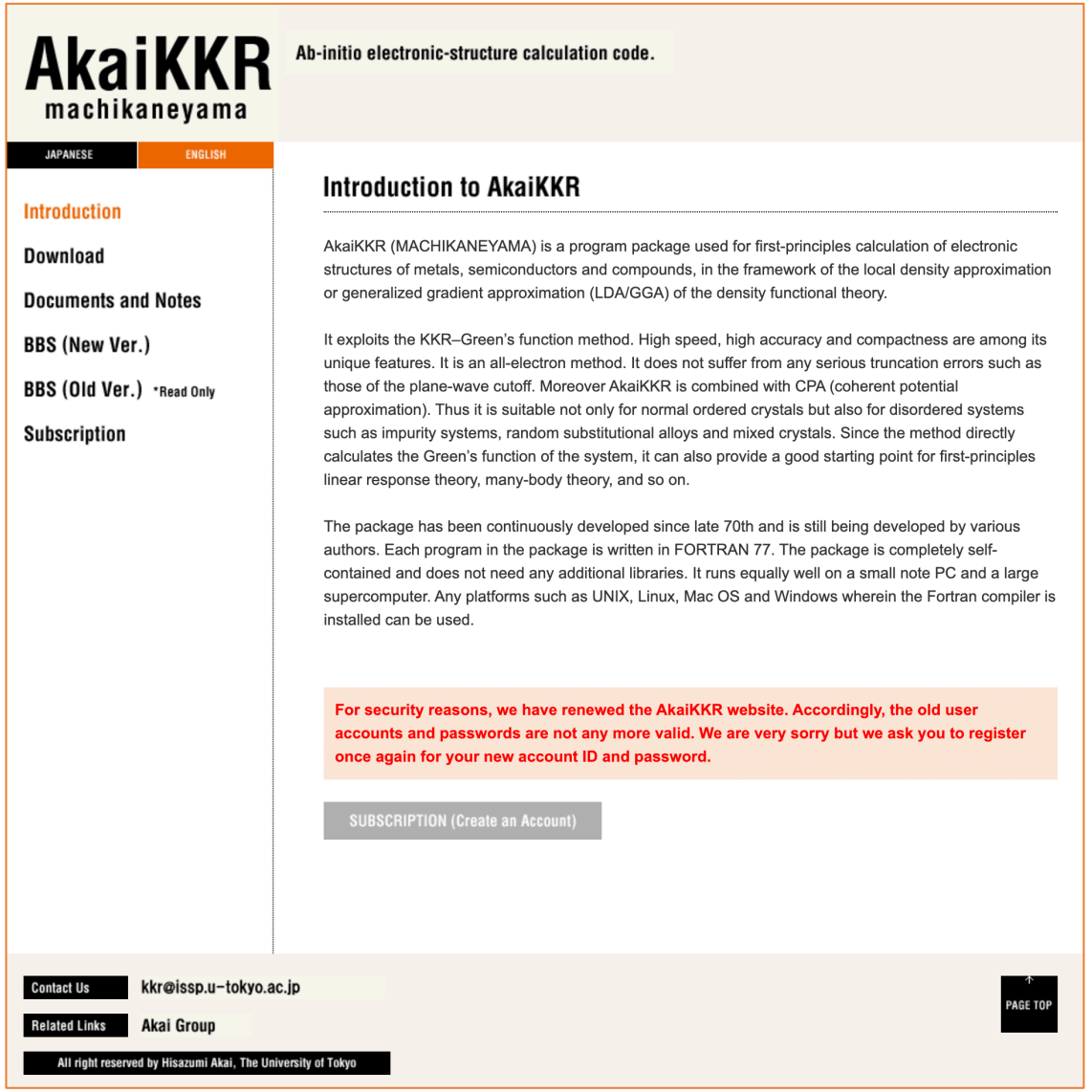
AkaiKKR

AkaiKKR: a software of DFT

- Green's function method (KKR method)
- Coherent Potential approximation (CPA)

Lastest ver：cpa2021v02gpu

http://kkr.issp.u-tokyo.ac.jp/



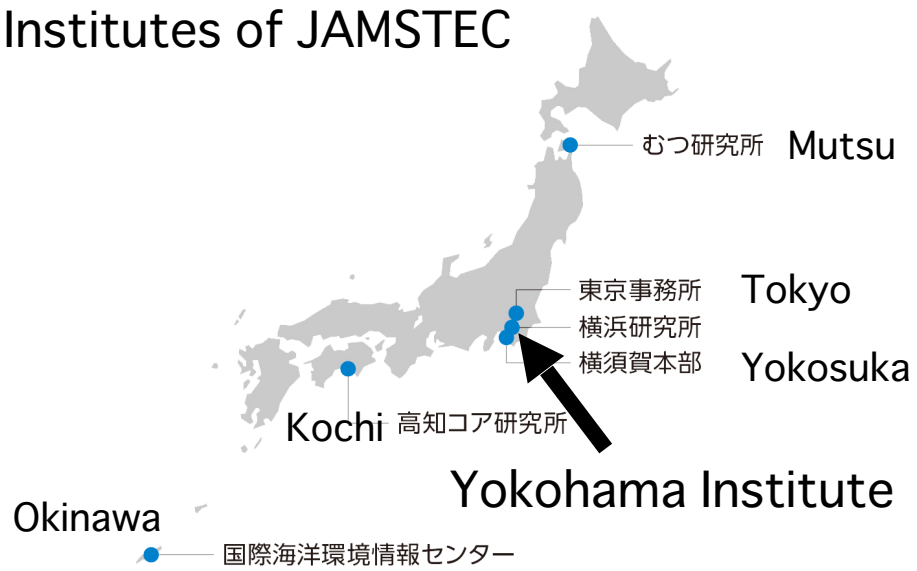
GPU-optimized program (Academeia Inc.)

1. Routine to generate Hamiltonian
2. Routine to solve Hamiltonian

Important literatures for AkaiKKR

[1] H. Akai, J. Phys. Soc. Jpn. 51, 468 (1982).
[2] K. Sato, et al., Rev. Mod. Phys. 82, 1633 (2010).
[3] T. Dietl, et al., Rev. Mod. Phys. 87, 1311 (2015).

Earth Simulator (ES4)



1st generation

40 TFlops
2002

2nd generation

131 TFlops
2009

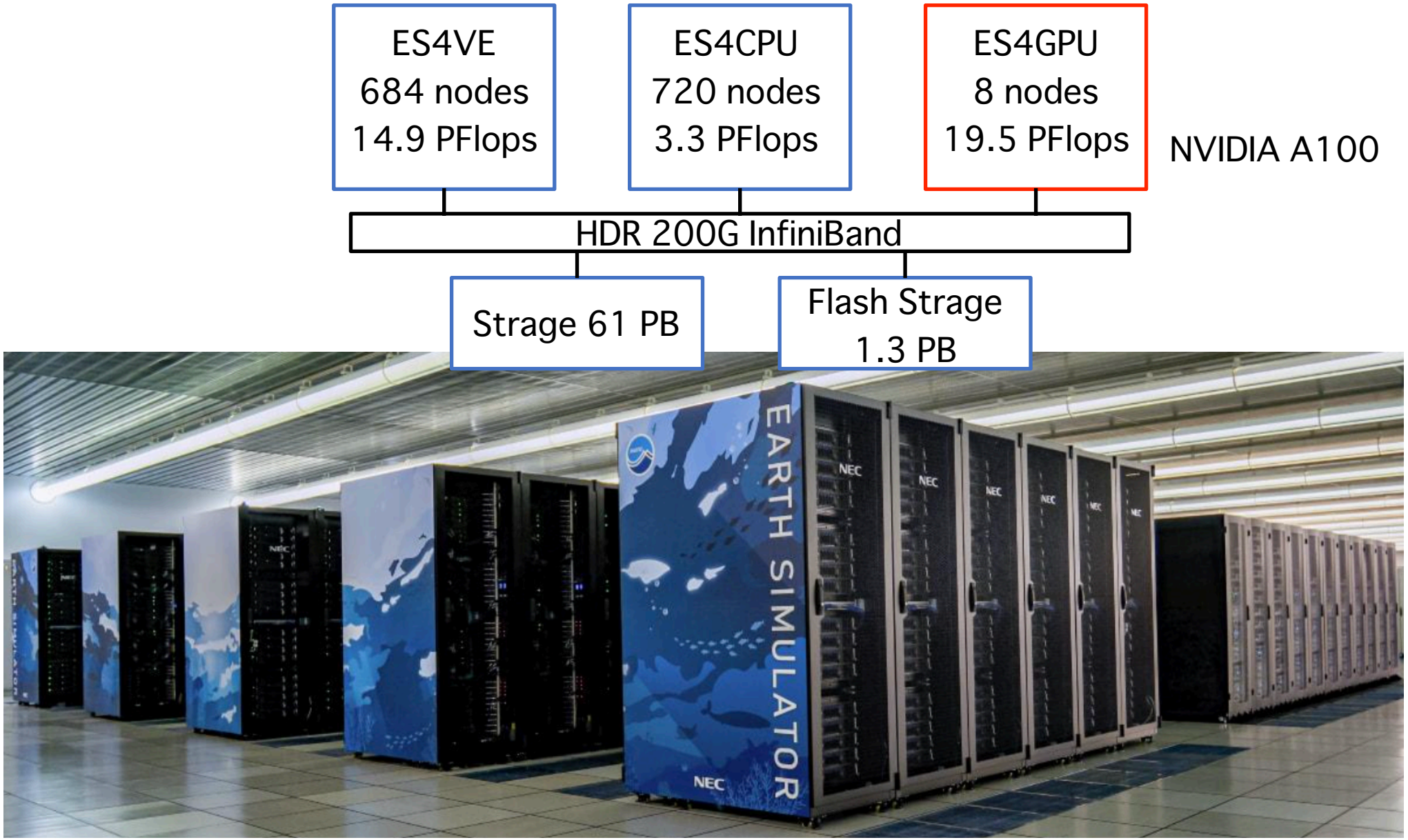
3rd generation

1.3 PFlops
2015

4th generation

19.5 PFlops
2021

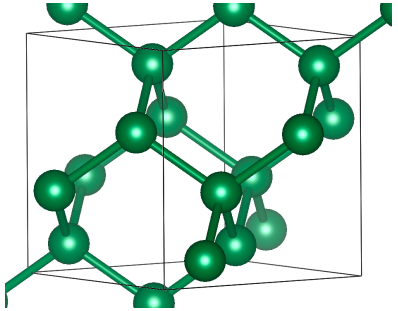
Earth Simulator (ES4)



Result 1: Dependence on the Number of Atoms

Si8 (FCC, Natom=16, bzqlty=6, Nonmagnetic state)

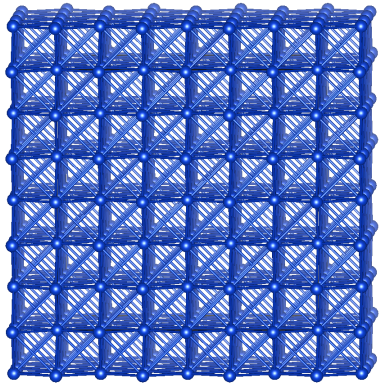
Architecture	Elapsed Time	Total energy (eV)
CPU	452.69 sec(=7.5 min)	-4613.3786 74633
GPU	101.88 sec(=1.7 min)	-4613.3786 74633



Silicon
a cubic lattice

Copper 108 (FCC, Natom=108, bzqlty=2, Nonmagnetic Metal)

Architecture	Elapsed Time	Total energy (eV)
CPU	6918.87 sec (=1.9 hours)	-353781.7339 40712
GPU	275.17 sec (=4.6 min)	-353781.7339 14122



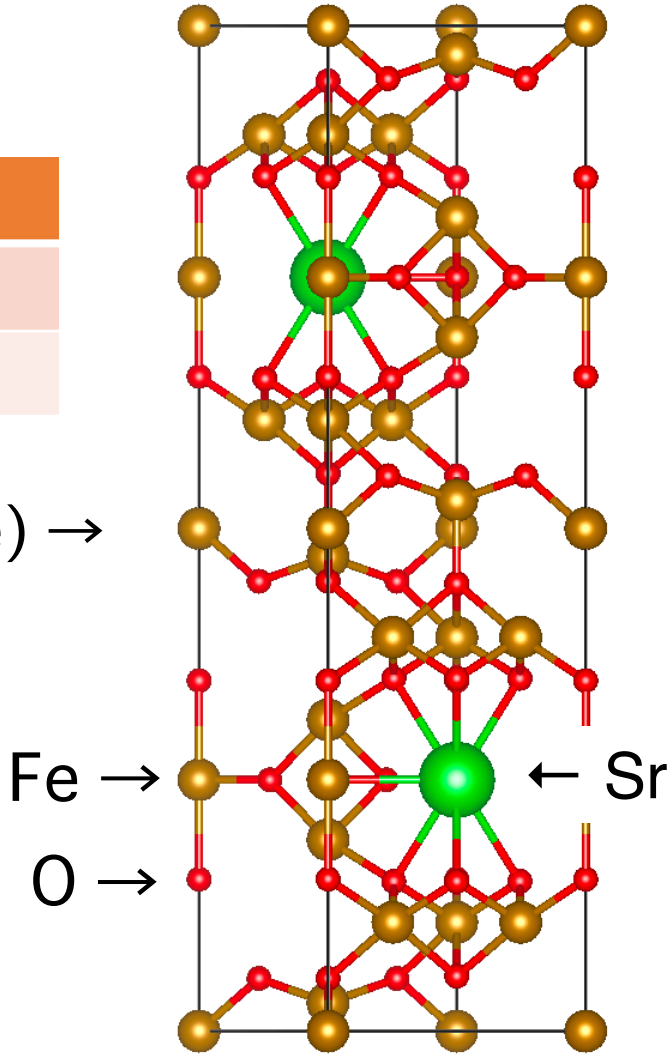
Copper
a cubic lattice

Result 2: Dependence on the Number of Atoms

Ferrite (Hexagonal SrFeO, Natom=64, bzqlty=3, Magnetic Insulator)

Architecture	Elapsed Time	Total energy (eV)
CPU	3801.95 sec (=1.1 hours)	-79352.7030 90297
GPU	675.29 sec (=11 min)	-79352.7030 91289

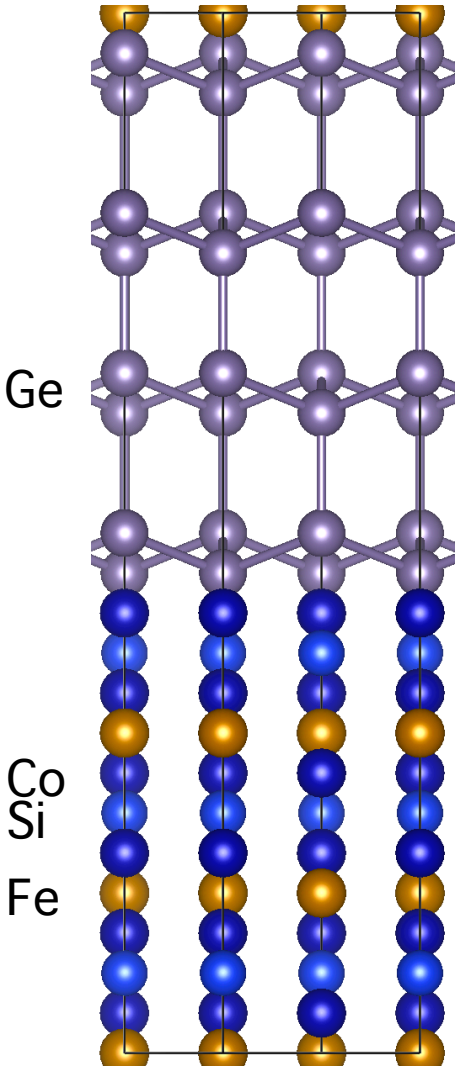
Ferrite (Hexagonal lattice) →



These results show that GPUs can be expected to achieve significantly better calculation performance than CPUs.

Result 3: an Interface Structure

Interface of Co_2FeSi and Ge, Natom=26, bzqlty=2, Magnetic metal / Semiconductor)



Architecture	Elapsed Time	Total energy (eV)
CPU	395.46 sec (=6.6 min)	not conv (maxiter=199)
GPU	92.70 sec (=1.5 min)	not conv (maxiter=199)
GPU	85.19 sec (=1.4 min)	-796772.489055 (iter=176)

↑ Convergence in a hyper-parameter, which is emrgn=0.2

Calculation time has been reduced in a single SCF loop.
Final calculation time depends on the number of loops.
Anyway, this calculation speed helps research activity.

Summary

- We have checked the performance of the quantum mechanics calculation using a software package of AkaiKKR on ES4GPU.
- The current results show that GPUs can be expected to achieve significantly better calculation performance than CPUs.
- Calculation time has been reduced in a single SCF loop.
- Total calculation times depend on the number of the loops.
- Anyway, this calculation speed helps our research activity.

Thank you very much for your kindly attention.