High Performance Computing Infrastructure (HPCI) and Software Development

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HPCI (High Performance Computing Infrastructure)

High-Performance Computing Infrastructure (HPCI) is a shared computational environment in Japan. The mission of HPCI is to realize the scientific and technological computing environment where a wide range of HPC users in Japan can access national HPC resources efficiently.

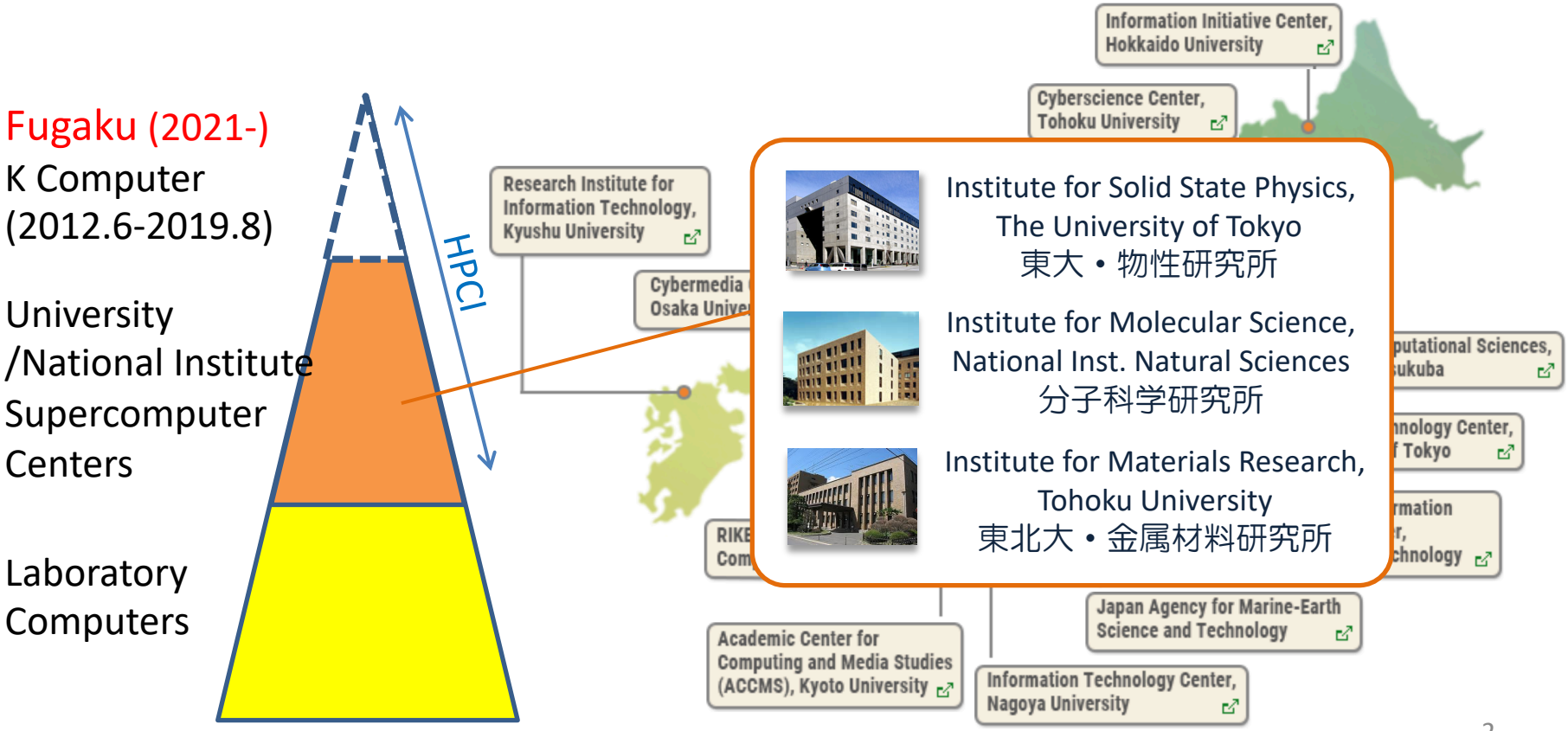
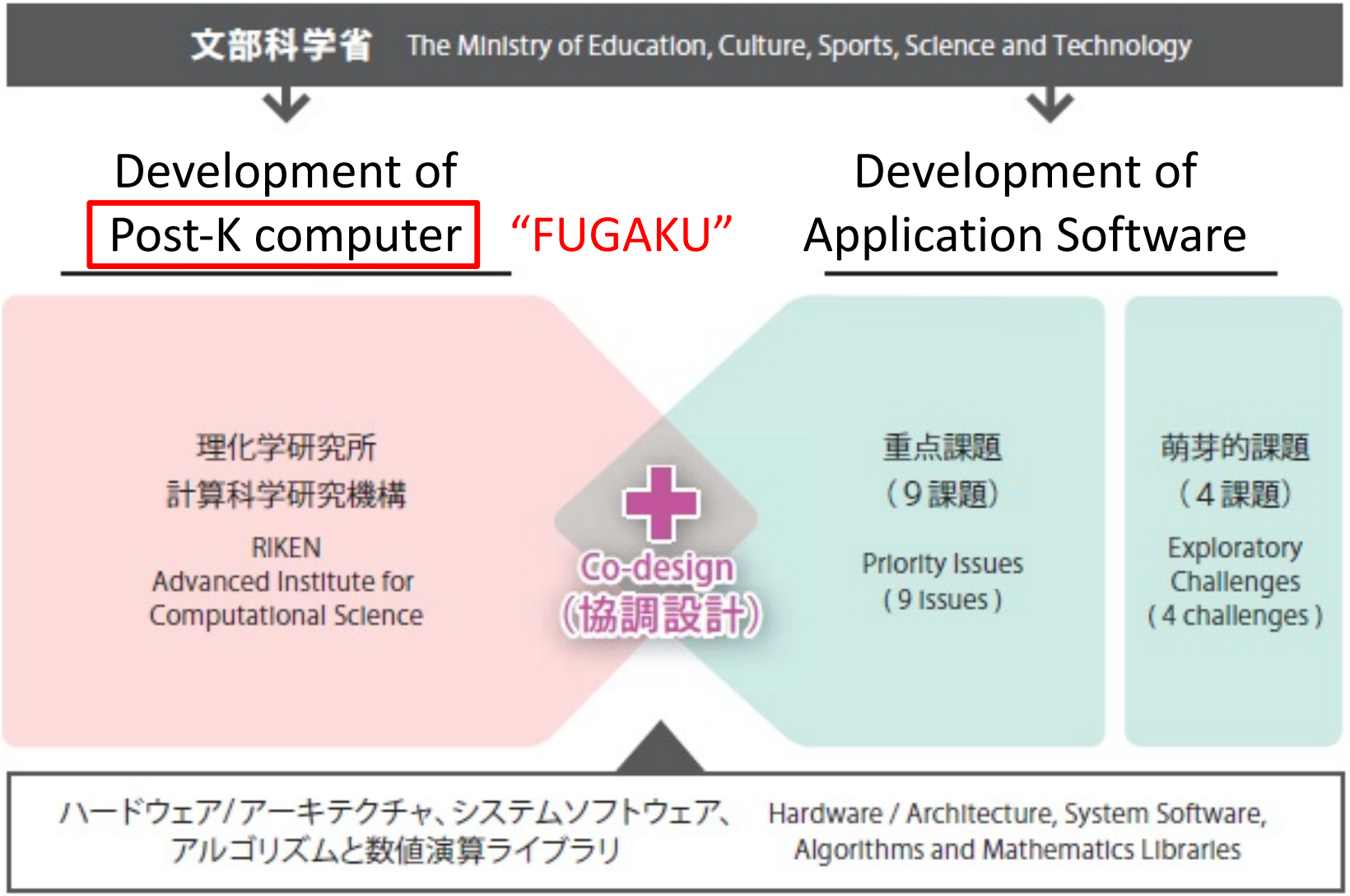


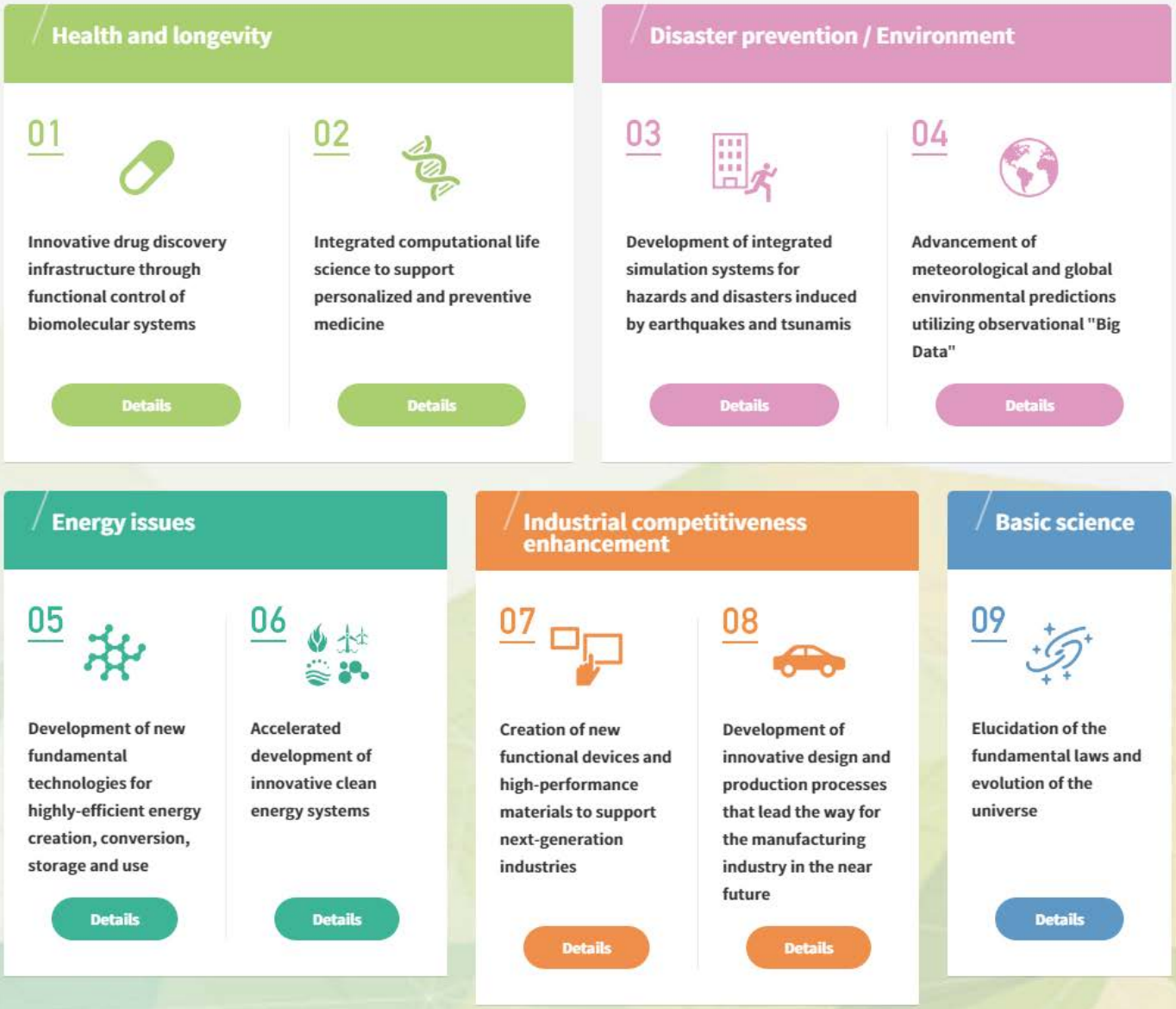
Figure 1: Organizations engaging in the HPCI system operation (Fiscal Year 2019)

FLAGSHIP 2020 Project (FY2015-2019)



http://www.aics.riken.jp/en/postk/project

9 priority issues in FLAGSHIP 2020 Project



http://www.aics.riken.jp/fs2020p/en/

CDMSI (FY2015-2019)

07

Creation of new functional
Devices and high-performance
Materials to
Support next-generation
Industries

http://www.aics.riken.jp/fs2020p/en/

The Institute for Solid State Physics,
the University of Tokyo

and 9 other institutes:
Institute for Materials Research (Tohoku Univ.), Institute for Molecular Science, University of Tsukuba, Osaka University, Nagoya University, Nagoya Institute of Technology, Yokohama National University, Tokyo University of Science, National Institute of Advanced Industrial Science and Technology

Sub-issues in CDMSI (FY2015-2019)

Methods

Sub-issue G: **Fundamental methods** for materials science simulation

Device

Sub-issue A: New-functionality and high-performance **semiconductor devices**

Sub-issue B: Unified **photonic-electronic devices**

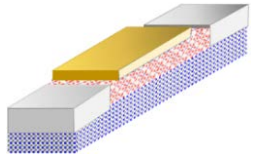
Sub-issue C: **Superconductors** and new functional devices and materials

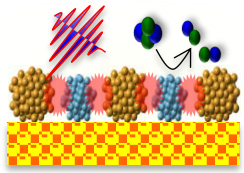
Materials

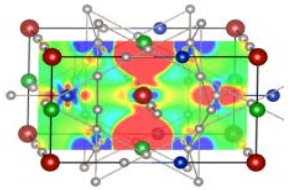
Sub-issue D: High performance permanent **magnets** and magnetic materials

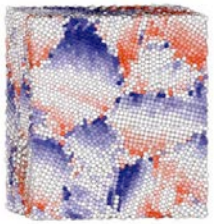
Sub-issue E: Advanced **structural materials**

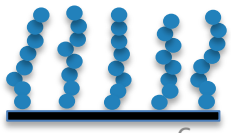
Sub-issue F: Next-generation functional **chemical substance**



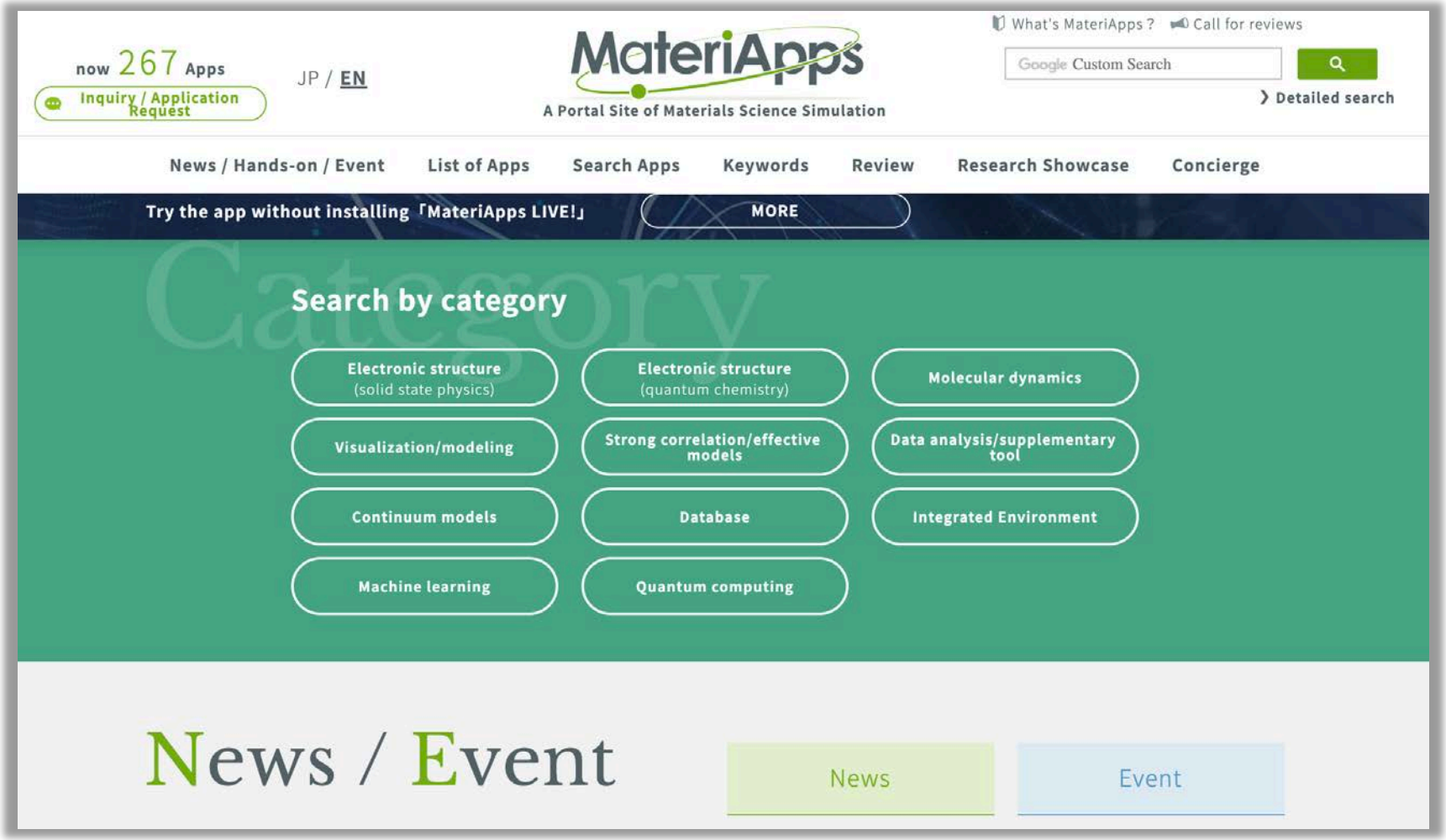








A portal site for materials science simulation



4300 users, >16000 pageview / month (FY2019)

2116 users, 11267 pageview / month (FY2018)

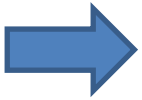
OpenMX

http://www.openmx-square.org

- A software package for electronic-structure calculation based on Density Functional Theory (DFT)
- Norm-conserving pseudopotentials
- Variationally optimized numerical atomic basis functions
- Besides basic functions, the package is equipped with
  - **O(N) method**
  - **Calculation of Magnetic anisotropy energy (MAE),**
  - **Exchange coupling parameters,**
  - **Z2 & Chern topological invariant,**
  - **Core level calculations for XPS**
  - **Interface with BoltzTrap**

  and many other functions

Main Contributor:
Taisuke Ozaki
(ISSP, U. Tokyo)



Magnetic Materials (ESICMM)
Structural Materials (ESISM)

Appendix

New features in OpenMX Ver. 3.9

Taisuke Ozaki (ISSP, Univ. of Tokyo)
Dec. 3, 2019

OpenMX Open source package for Material eXplorer

- Software package for density functional calculations of molecules and bulks
- Norm-conserving pseudopotentials (PPs)
- Variationally optimized numerical atomic basis functions

Basic functionalities

- SCF calc. by LDA, GGA, DFT+U
- Total energy and forces on atoms
- Band dispersion and density of states
- Geometry optimization by BFGS, RF, EF
- Charge analysis by Mullken, Voronoi, ESP
- Molecular dynamics with NEV and NVT ensembles
- Charge doping
- Fermi surface
- Analysis of charge, spin, potentials by cube files
- Database of optimized PPs and basis funcitons

Extensions

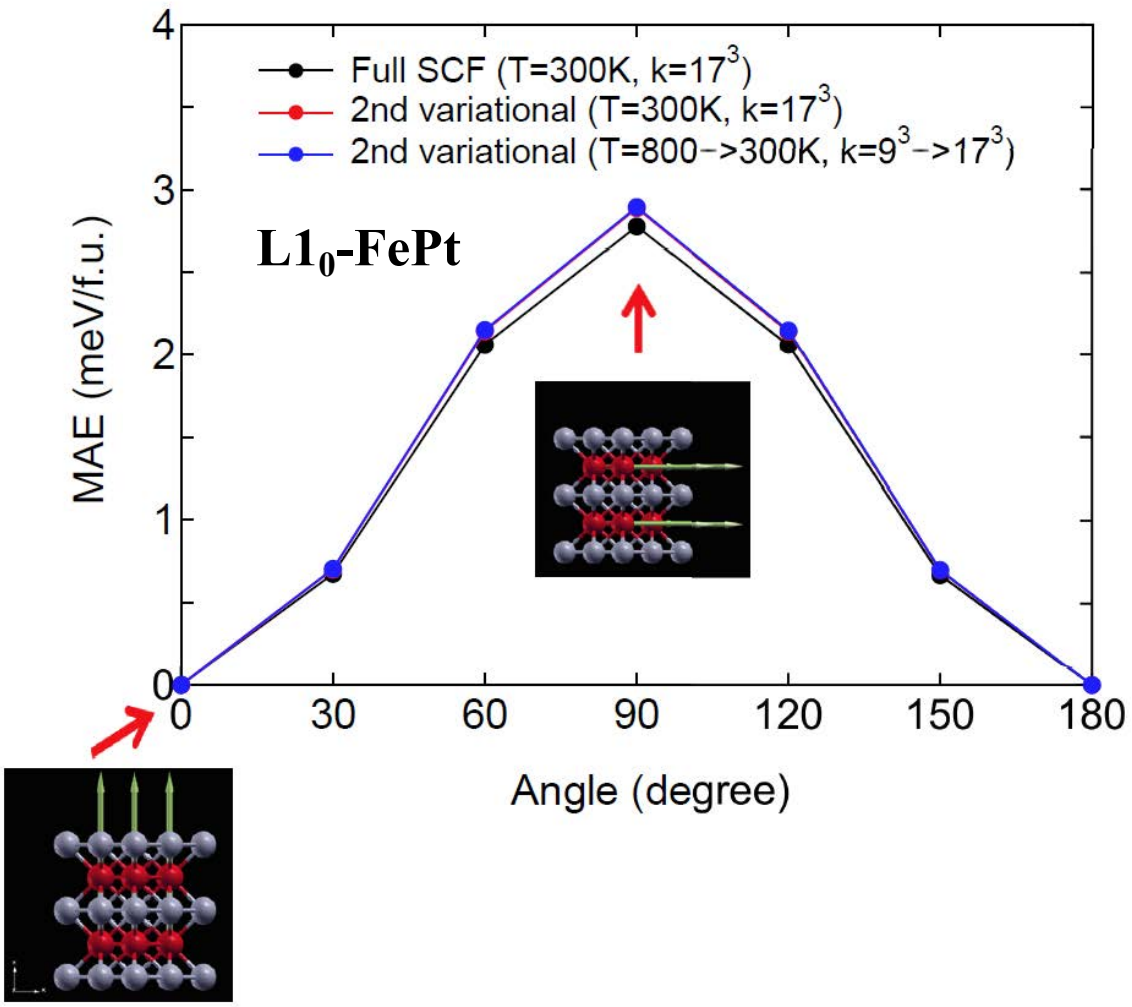
- O(N) and low-order scaling diagonalization
- Non-collinear DFT for non-collinear magnetism
- Spin-orbit coupling included self-consistently
- Electronic transport by non-equilibrium Green function
- Electronic polarization by the Berry phase formalism
- Maximally localized Wannier functions
- Effective screening medium method for biased system
- Reaction path search by the NEB method
- Band unfolding method
- STM image by the Tersoff-Hamann method
- etc.

New features in OpenMX Ver. 3.9

- Database 2019 of PAO and VPS (Ozaki)
- Database 2019 of PAO and VPS for core level excitation (Ozaki)
- Core level calculations for XPS (Ozaki)
- O(N) DC-LNO method (Ozaki)
- Calculations of gaseous charged systems (Ozaki)
- Complex dielectric function & optical conductivity tensors (YTL)
- Spin texture for Rashba effect (Kotaka, Yamaguchi, Ishii)
- Generalized Bloch theorem for spin spiral (Prayitno, Ishii)
- Z2 & Chern topological invariant (Sawahata, Ishii)
- Improvement of polB (Yamaguchi)
- Second variational scheme of SOI (Po-Hao Chang)
- Efficient implementation of j_{ij} (Terasawa)
- Optimization of enthalpy (Ozaki)
- New DFT+U functionals (Ryee&Han)
- Mixing methods of DIISV (Ozaki)
- ELPA1/ELPA2 (Duy and Ozaki)
- OpenMX engine by MPI_spawn (Ozaki)
- Jx (Yoon, Kim, Sim, Han)
- Interface with FermiSurfer (Kawamura)
- Interface with BoltzTrap (Miyata)
- Interface with ASE (Yu)

Second variational scheme for evaluation of magnetic anisotropy energy (MAE) supported by P.-H. Chang and Ozaki

A second variational method is supported to calculate band structures modified with spin-orbit coupling (SOI) and magnetic anisotropy energy (MAE).

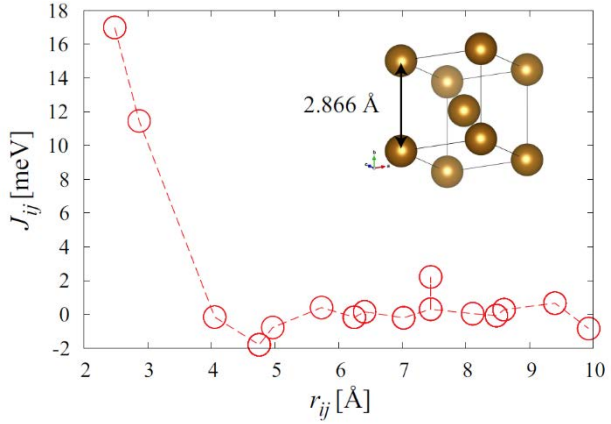


Second variational scheme

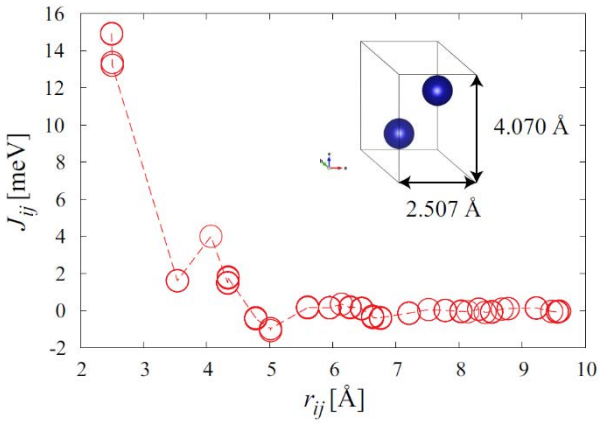
- First, the SCF calculation is performed by the collinear DFT
- Second, with the SCF charge the one-shot diagonalization is performed with SOI.
- The total energy is evaluated by the Harris functional.

Efficient calculations of exchange coupling parameters supported by Terasawa, Ozaki, and Gohda

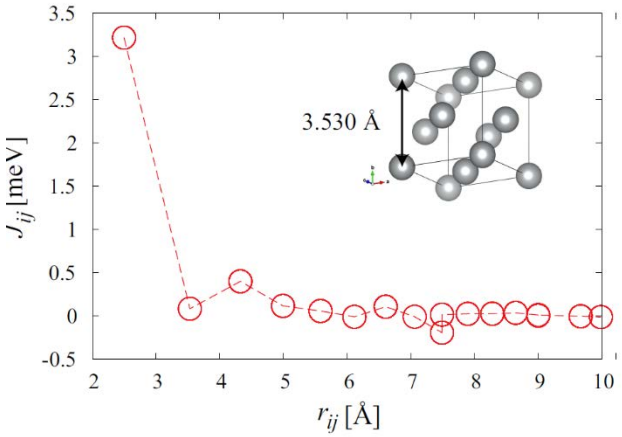
A post-processing code 'jx' to calculate exchange coupling parameters J_{ij} has been largely improved so that the individual J_{ij} in bulks can be calculated efficiently using a contour integration method.



(a) bcc Fe, k-grid = 27×27×27



(b) hcp Co, k-grid = 32×32×20



(c) fcc Ni, k-grid = 24×24×24

Currie temperature

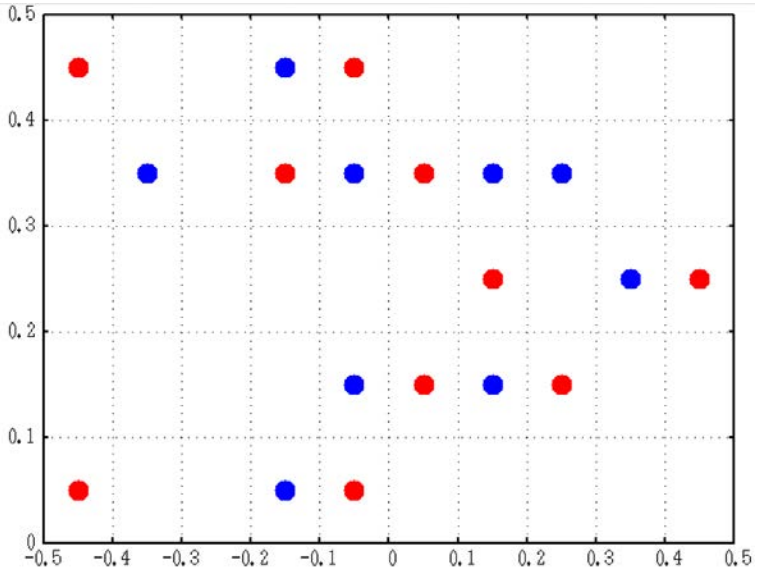
System	T_C [K] calculated	T_C [K] experimental
bcc Fe	1321	1040
hcp Co	1640	1131
fcc Ni	445	627

A Terasawa, M Matsumoto, T Ozaki, and Y Gohda, J. Phys. Soc. Jpn. **88**, 114706 (2019).

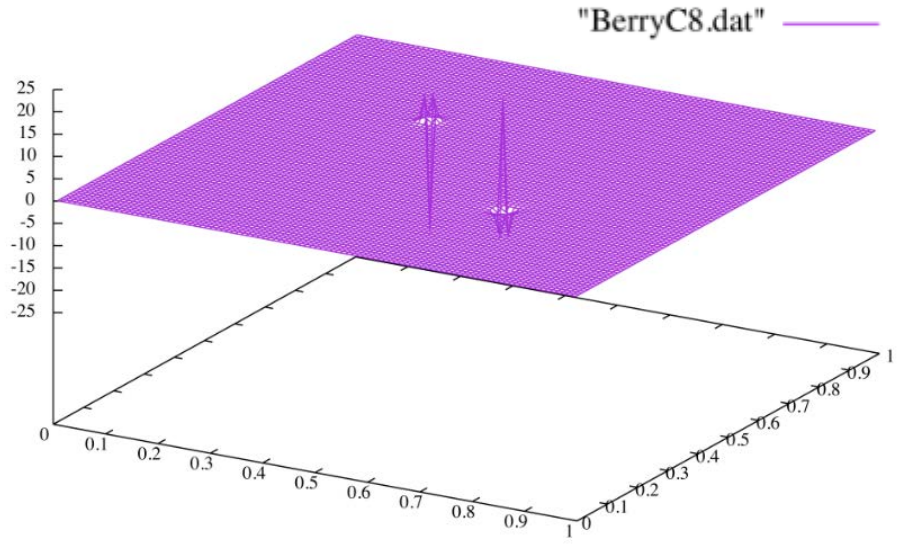
Chern number, Berry curvature, and Z_2 invariant supported by Sawahata and Ishii

In OpenMX Ver. 3.9, a post-processing code 'calB' is supported to calculate the Chern number and Berry curvature of bands using overlap matrix elements between Kohn-Sham orbitals at neighboring k-points by the Fukui-Hatsugai-Suzuki method. The Chern number is a topological invariant being an integer number, which characterizes the topology of bands for any materials. We also release another post-processing code 'Z2FH' to calculate the Z_2 topological invariant using the Berry phase by the Fukui-Hatsugai method.

An example for the calculation of integer-valued field Bi_2Se_3



Berry curvature for bands of graphene



H. Sawahata, N. Yamaguchi, H. Kotaka, and F. Ishii, Jpn. J. Appl. Phys. 57, 030309 (2018).

Absolute binding energies of core levels
XPS core level energies supported by Ozaki

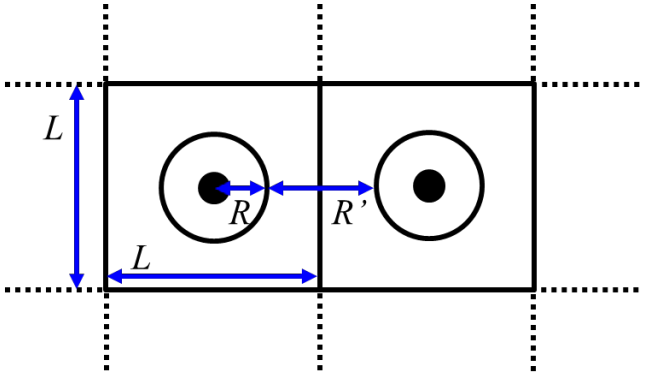
A general method has been supported to calculate absolute binding energies of core levels in metals and insulators, based on a penalty functional and an exact Coulomb cutoff method in the framework of density functional theory. With the method one can treat multiple splittings due to chemical shift, spin-orbit coupling, and exchange interaction on equal footing.

$$E_{\mathrm{b}} = E_{\mathrm{f}}^{(0)}(N-1) - E_{\mathrm{i}}^{(0)}(N) + \mu_0$$

Penalty functional

$$E_{\mathrm{f}} = E_{\mathrm{DFT}} + E_{\mathrm{p}}$$

Exact Coulomb cutoff method



Material	State	Calc. (eV)	Expt. (eV)
Gapped system			
c-BN	N-1s	398.87	398.1*
bulk NH_3	N-1s	398.92	399.0$^+$
Diamond	C-1s	286.50	285.6†
Si	Si-2$p_{1/2}$	100.13	99.8*
Si	Si-2$p_{3/2}$	99.40	99.2*
Semimetal or Metal			
Graphene	C-1s	284.23	284.4†
TiN	N-1s	396.43	397.1§
TiC	C-1s	281.43	281.5*

Mean absolute error: 0.4 eV, Mean relative error: 0.16 %

T. Ozaki and C.-C. Lee, Phys. Rev. Lett. 118, 026401 (2017)

Interface with BoltzTrap supported by Miyata

OpenMX is interfaced with BoltzTraP which calculates electron transport coefficients based on the Boltzmann theory from the wave number dependence of the energy eigenvalues in the Kohn-Sham equation. The interface with BoltzTraP enables us to calculate physical properties such as the Seebeck coefficient, electrical conductivity, electronic thermal conductivity, and the Hall coefficient. The functionality is compatible with not only the collinear calculations, but also the non-collinear calculations.

M. Miyata et al., Journal of Electronic Materials 47, 3254 (2017).

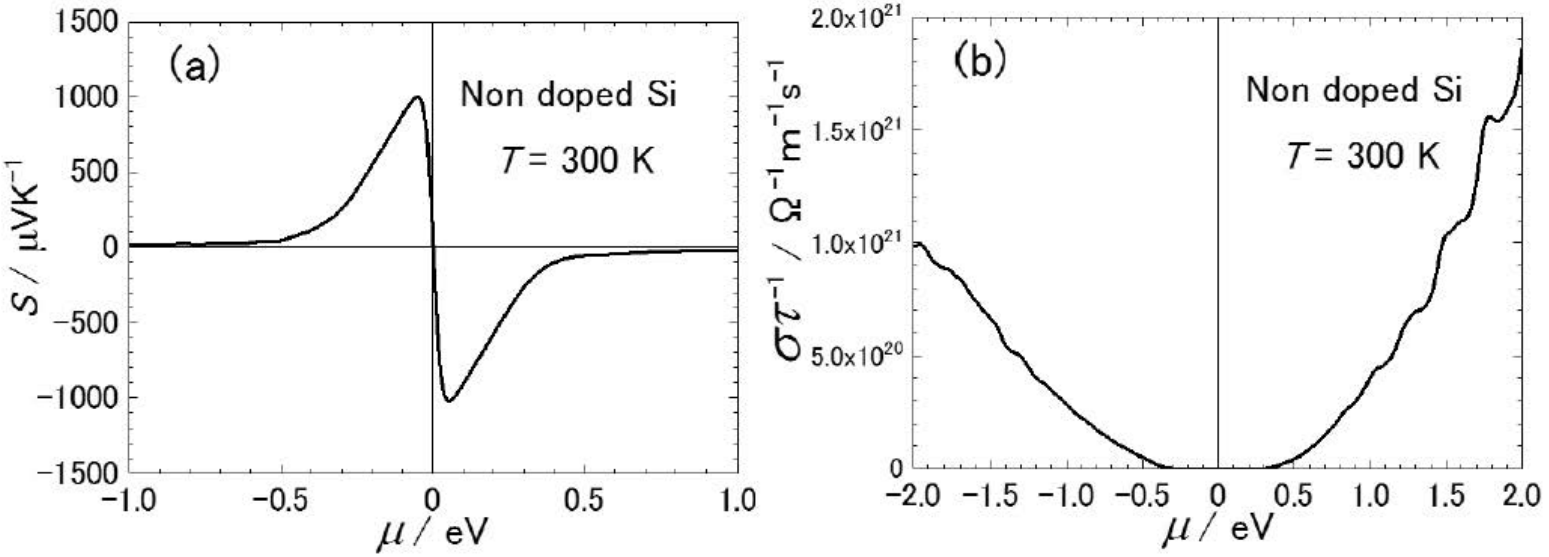


Figure 78: (a) Seebeck coefficient S, and (b) the electric conductivity $\sigma\tau_{\mathrm{el}}^{-1}$ of non-doped Si in the diamond structure as a function of the chemical potential at 300 K obtained by OpenMX and BoltzTraP. The Fourier interpolation factor was set to 25. The input file 'Si_BoltzTraP.dat' used for the calculation is available in the directory 'work'.