New features in OpenMX Ver. 3.9

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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.

History of OpenMX

2000 Start of development

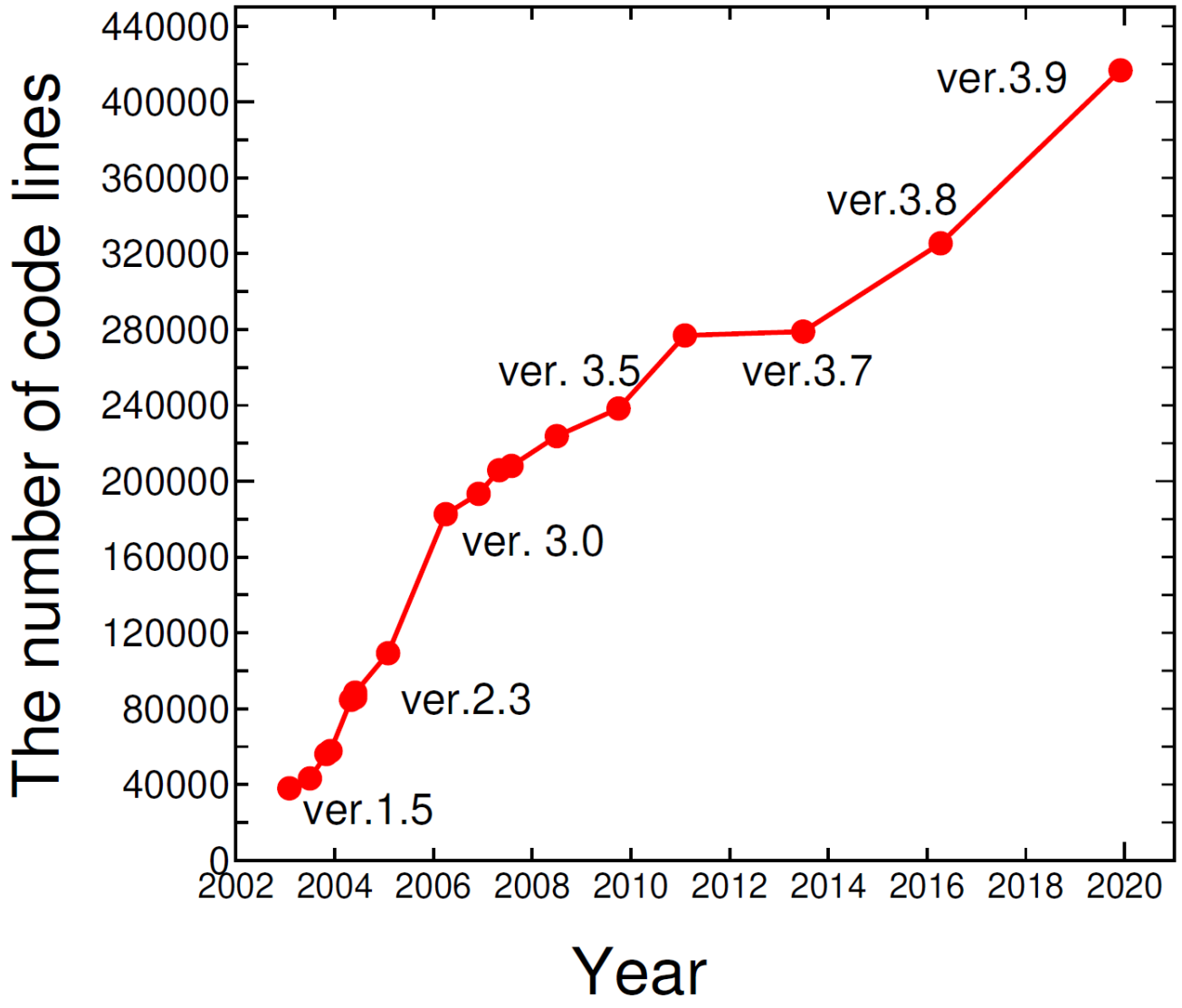
2003 Public release (GNU-GPL)

2003 Collaboration:
AIST, NIMS, SNU
KAIST, JAIST,
Kanazawa Univ.
CAS, UAM
NISSAN, Fujitsu Labs.
etc.

2019 19 public releases
Latest version: 3.9

http://www.openmx-square.org

Development of OpenMX code



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Materials studied by OpenMX

First characterization of silicene on ZrB_2 in collaboration with experimental groups

A. Fleurence et al., Phys. Rev. Lett. 108, 245501 (2012).

First identification of Jeff=1/2 Mott state of Ir oxides

B.J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008).

Theoretical proposal of topological insulators

C.-H. Kim et al., Phys. Rev. Lett. 108, 106401 (2012).
H. Weng et al., Phy. Rev. X 4, 011002 (2014).

First-principles molecular dynamics simulations for Li ion battery

T. Ohwaki et al., J. Chem. Phys. 136, 134101 (2012).
T. Ohwaki et al., J. Chem. Phys. 140, 244105 (2014).

Magnetic anisotropy energy of magnets

Z. Torbatian et al., Appl. Phys. Lett. 104, 242403 (2014).
I. Kitagawa et al., Phys. Rev. B 81, 214408 (2010).

Electronic transport of graphene nanoribbon on surface oxidized Si

H. Jippo et al., Appl. Phys. Express 7, 025101 (2014).
M. Ohfuchi et al., Appl. Phys. Express 4, 095101 (2011).

Interface structures of carbide precipitate in bcc-Fe

H. Sawada et al., Modelling Simul. Mater. Sci. Eng. 21, 045012 (2013).

Universality of medium range ordered structure in amorphous metal oxides

K. Nishio et al., Phys. Rev. Lett. 340, 155502 (2013).

Materials treated so far

Silicene, graphene
Carbon nanotubes
Transition metal oxides
Topological insulators
Intermetallic compounds
Molecular magnets
Rare earth magnets
Lithium ion related materials
Structural materials
etc.

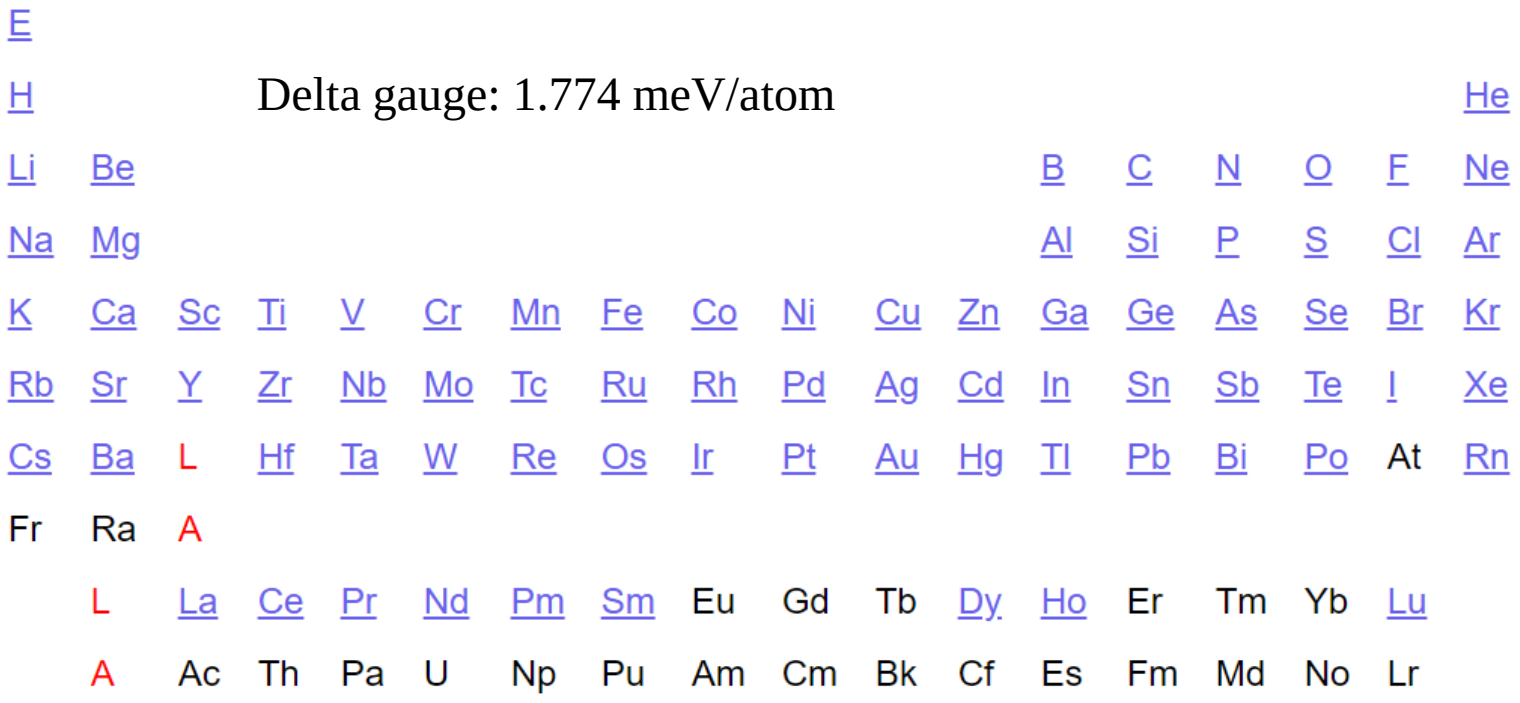
About 700 published papers

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)

Database 2019 of PAO and VPS supported by Ozaki

The database of fully relativistic pseudopotentials (VPS) and optimized pseudo-atomic orbitals (PAO) files has been updated as Database (2019), and distributed with OpenMX Ver. 3.9. Though the most of data are the same as in Ver. 2013, the VPS and PAO files for Fe, Os, Tc, La, Ce, Pr, and Pm are updated. The mean delta gauge of 71 elements in the database Ver. 2019 is 1.774 meV/atom with the standard deviation of 1.702 meV/atom.



https://t-ozaki.issp.u-tokyo.ac.jp/vps_pao2019/

Database 2019 for core level excitations supported by Ozaki

The database of fully relativistic pseudopotentials (VPS) and pseudo-atomic orbitals (PAO) which can be used for calculations of core level excitations has been released as Database (2019) for core excitations. The data for B, C, N, O, Si, S, Ge, Pt elements are available. When you calculate absolute binding energies of core levels in bulk and gaseous systems, which can be measured in X-ray photoemission spectroscopy (XPS), the VPS and PAO files have to be used.

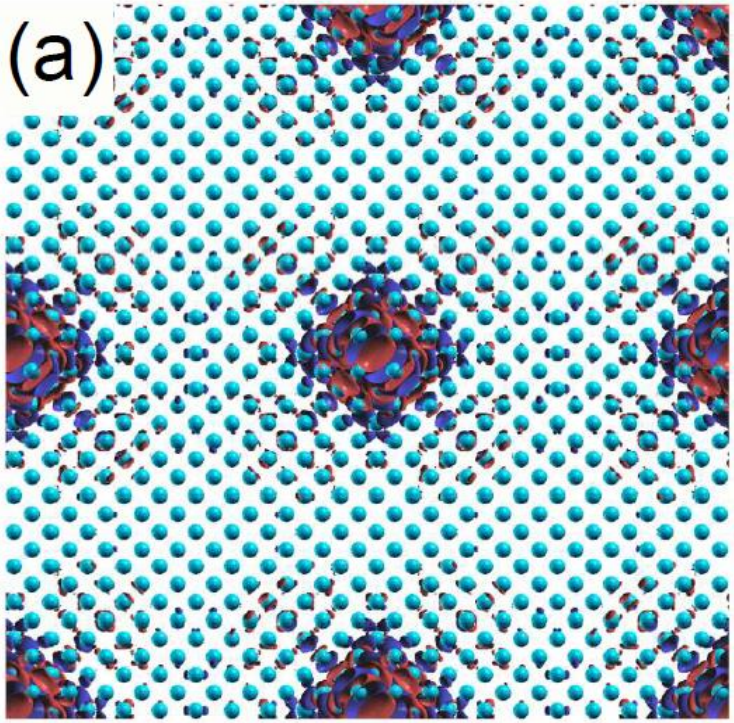
These PAO and VPS can be utilized for simulation of core level excitations such as XPS and XAS.

E																
H																He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	A															
	L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
	A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

https://t-ozaki.issp.u-tokyo.ac.jp/vps_pao_core2019/

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.

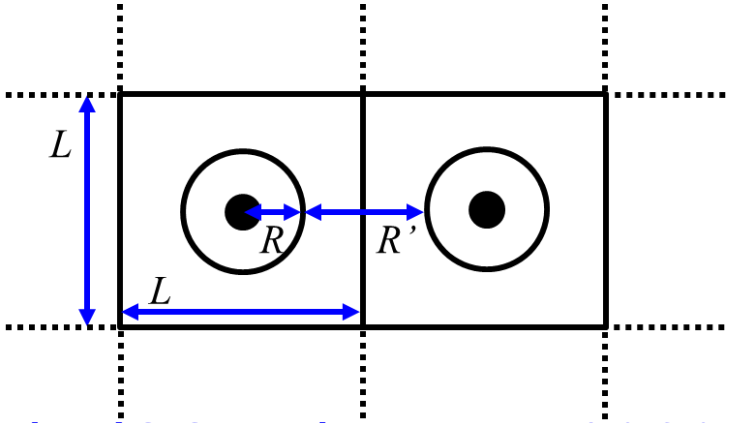


$$E_{\mathrm{b}} = E_{\mathrm{f}}^{(0)}(N-1) - E_{\mathrm{i}}^{(0)}(N) + \mu_0$$

Penalty functional

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

Exact Coulomb cutoff method



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

Absolute values: Expt. vs. Calcs. for solids

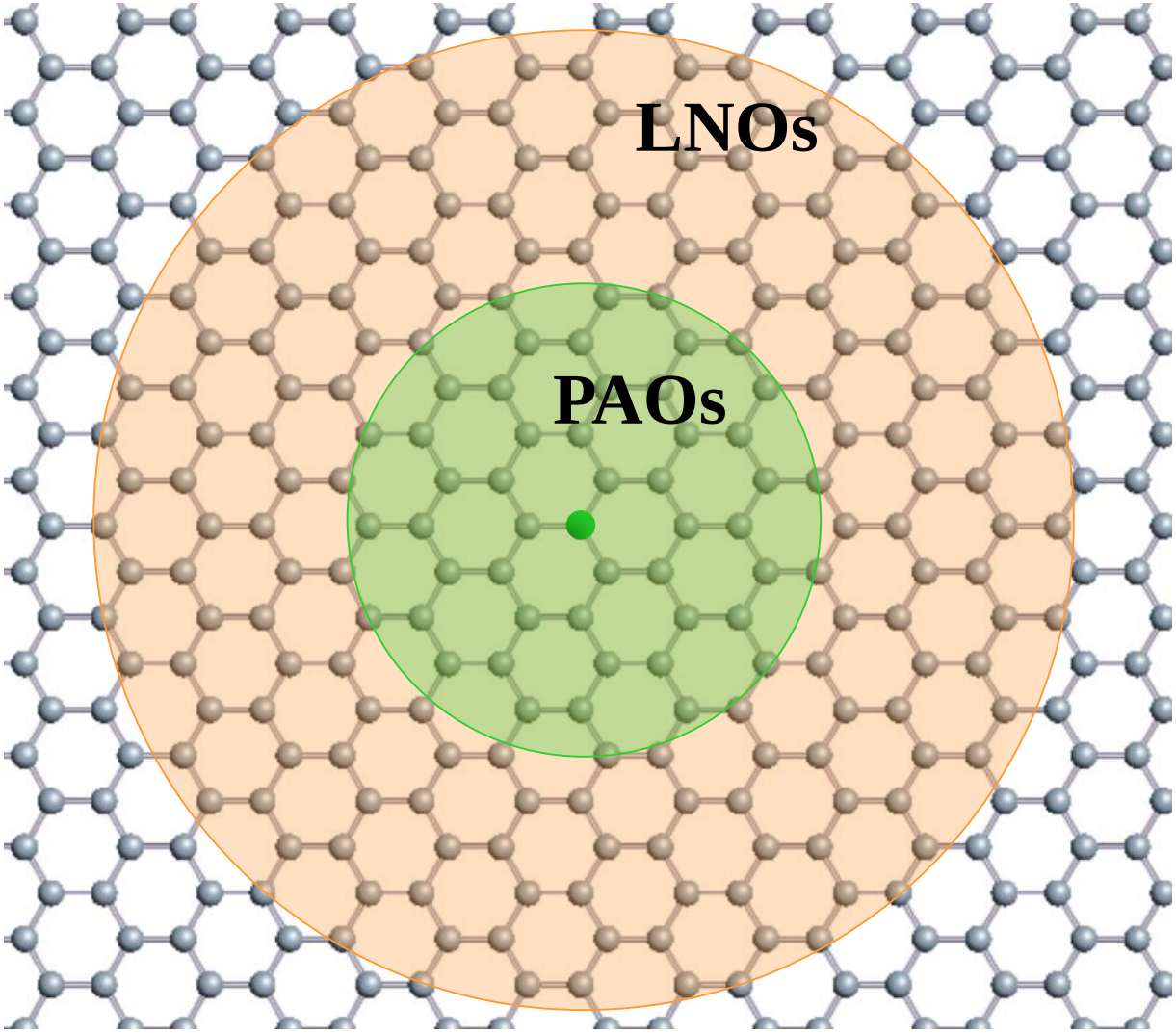
Material	State	Calc. (eV)	Expt. (eV)
Gapped system			
c-BN	N-1s	398.87	398.1*
bulk NH_3	N-1s	398.92	399.0$^+$
Diamond	C-1s	286.50	285.6†
Si	Si-2$p_{1/2}$	100.13	99.8*
Si	Si-2$p_{3/2}$	99.40	99.2*
Semimetal or Metal			
Graphene	C-1s	284.23	284.4†
TiN	N-1s	396.43	397.1§
TiC	C-1s	281.43	281.5*

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

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

O(N) DC method with LNOs supported by Ozaki

An efficient O(N) divide-conquer (DC) method based on localized natural orbitals (LNOs) has been released for large-scale DFT calculations of gapped and metallic systems.



Algorithms:

(1) Calculate LNOs for all the atoms.

↓

(2) MPI communicate LNOs

↓

(3) Construct a local H and S with PAOs and LNOs.

↓

(4) Solve a generalized eigenvalue problem for each atom.

↓

(5) Find a common μ.

↓

(6) Calculate density matrix and charge density.

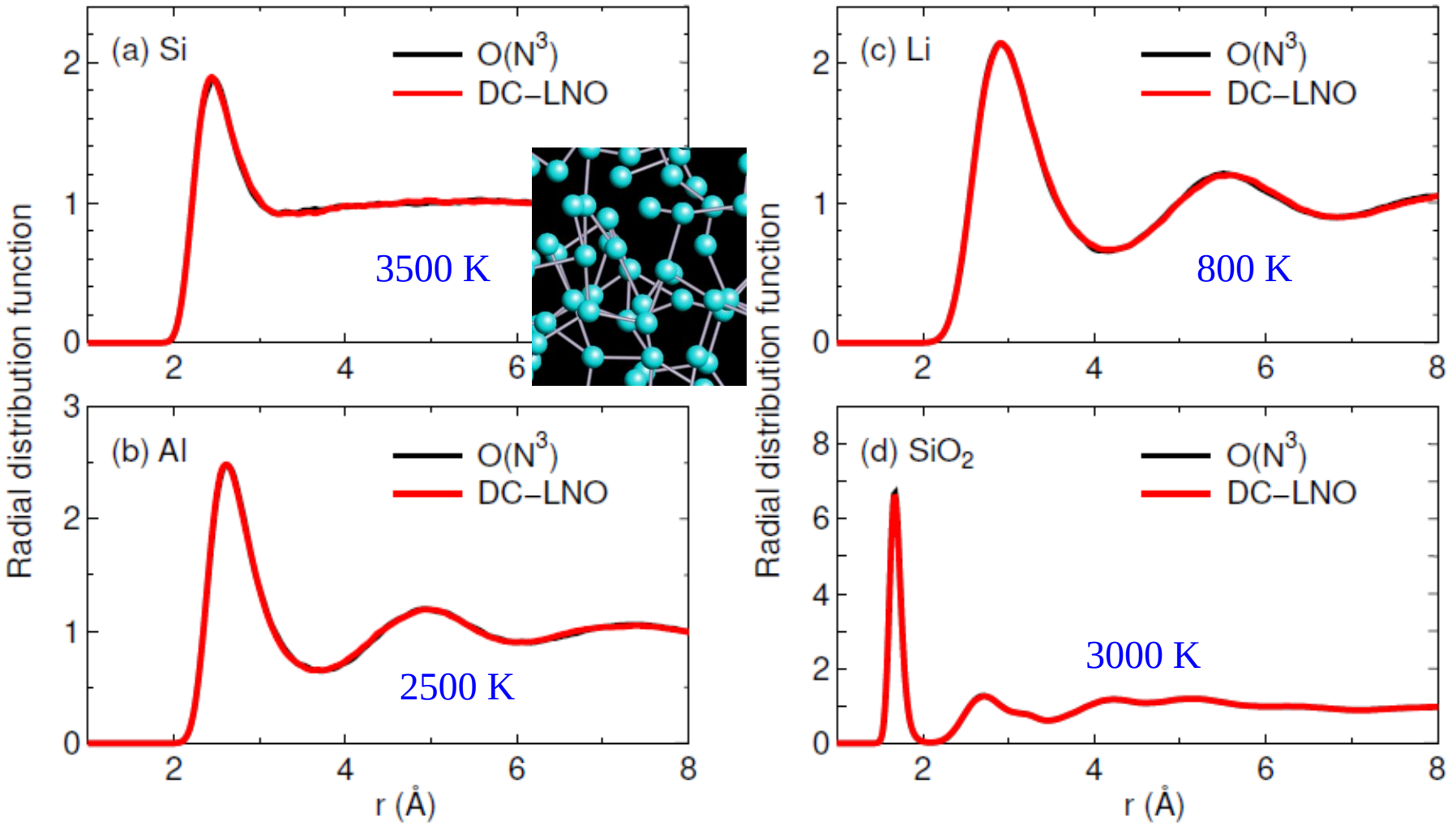
↓

Until SCF go to (1).

T. Ozaki, M. Fukuda, and G. Jiang, Phys. Rev. B 98, 245137 (2018).

Radial distribution functions in liquids

The DC-LNO method well reproduces the results by O(N^3) method.



T. Ozaki, M. Fukuda, and G. Jiang, Phys. Rev. B 98, 245137 (2018).

Calculations of gaseous charged systems supported by Ozaki

The ionization potential and electron affinity of gaseous systems can be calculated by a delta SCF method with an exact Coulomb cutoff method.

Ionization potential

System	Expt. (eV)	Calc. (eV)	Input files
H_2O	12.65 [92]	12.69	H2O+0.dat, H2O+1.dat
C_2H_2	11.43 [93]	11.47	C2H2+0.dat, C2H2+1.dat
C_2H_2	10.55 [93]	10.57	C2H4+0.dat, C2H4+1.dat
O_2	12.04 [93]	12.85	O2+0.dat, O2+1.dat
CO	14.01 [93]	13.85	CO+0.dat, CO+1.dat

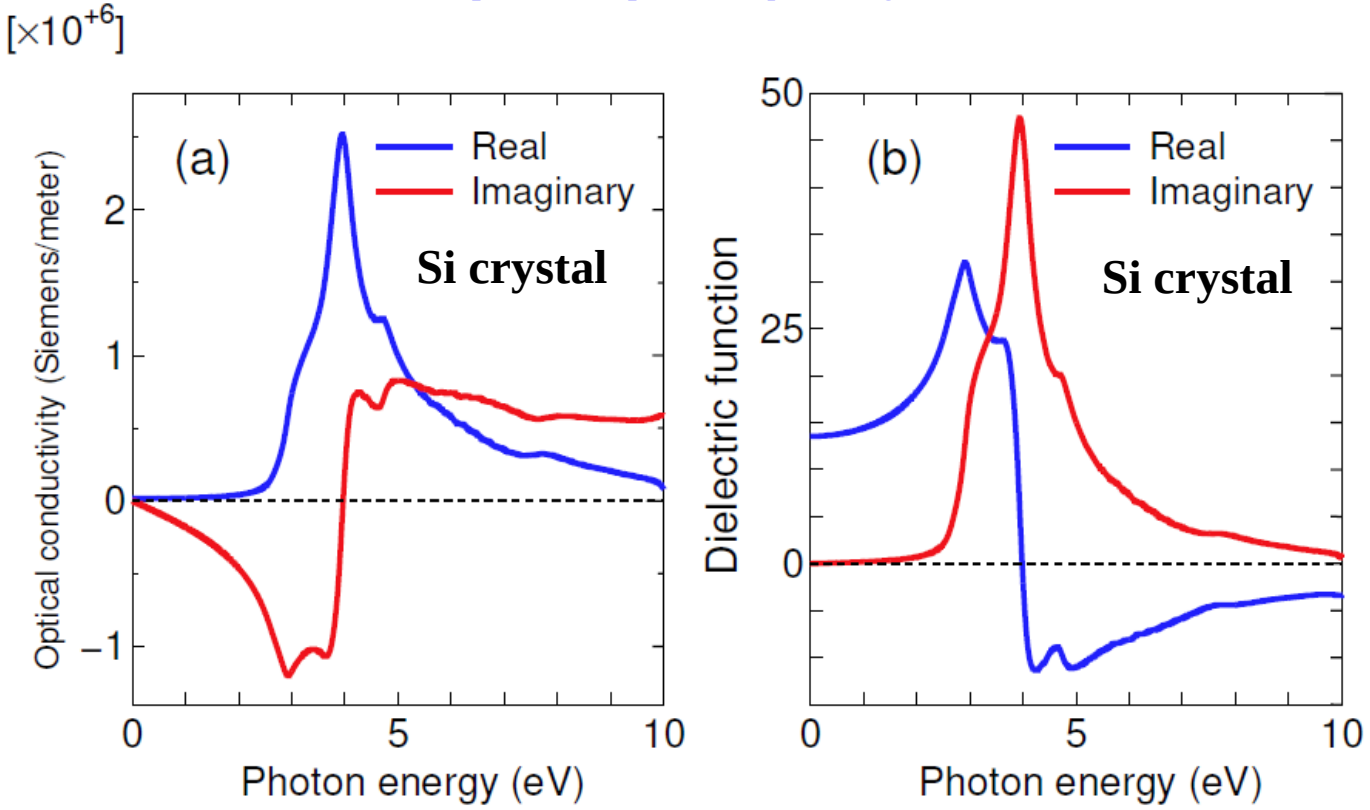
Electron affinity

System	Expt. (eV)	Calc. (eV)	Input files
OH	1.81 [93]	1.82	OH-0.dat, OH-1.dat
O_2	0.41 [93]	-0.29	O2-0.dat, O2-1.dat
Cl_2	2.37 [93]	0.96	Cl2-0.dat, Cl2-1.dat
CN	3.88 [93]	3.51	CN-0.dat, CN-1.dat
SiH	1.27 [93]	1.17	SiH-0.dat, SiH-1.dat

Dielectric function and optical conductivity supported by Y.-T. Lee and Ozaki

The conductivity and dielectric function can be calculated based on the Kubo-Greenwood formula. Starting from the Born approximation, the complex tensor of conductivity and dielectric function, which are frequency dependent, are calculated within a linear response to the ground state. Other physical quantities such as absorption, extinction, transmission, reflection, and refractive index are also calculated, which are all derived from the conductivity.

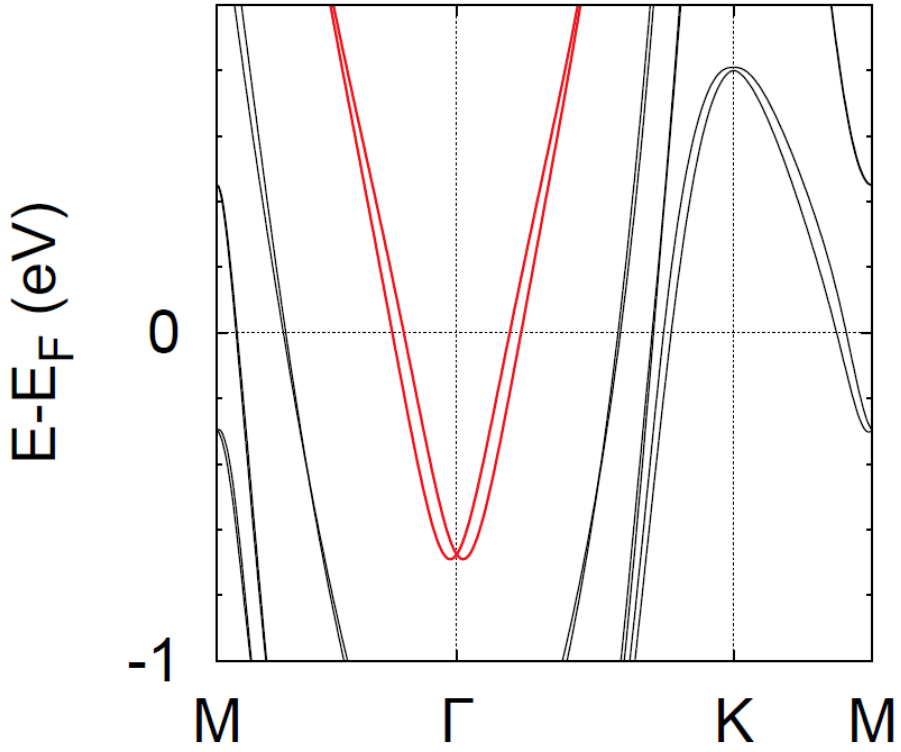
http://www.openmx-square.org/tech_notes/Dielectric_Function_YTL.pdf



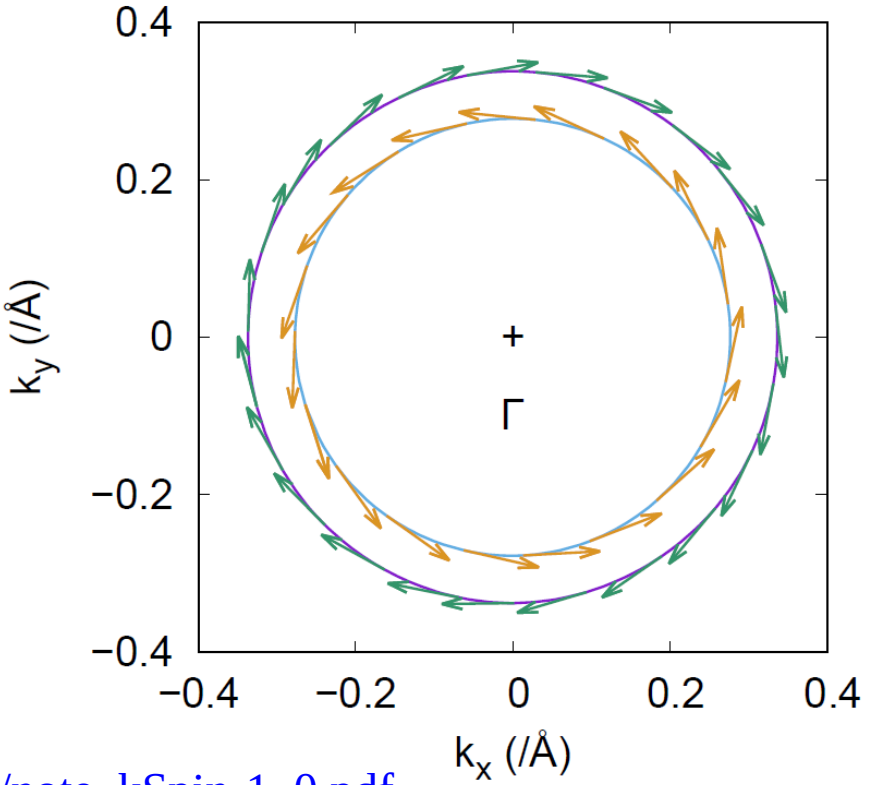
Spin texture analysis in Rashba splitting supported by Kotaka, Yamaguchi, and Ishii

The spin texture can be analyzed in the case of a non-collinear calculation with spin-orbit coupling.

Band structure for the Rashba spin splitting at the Au(111) surface.



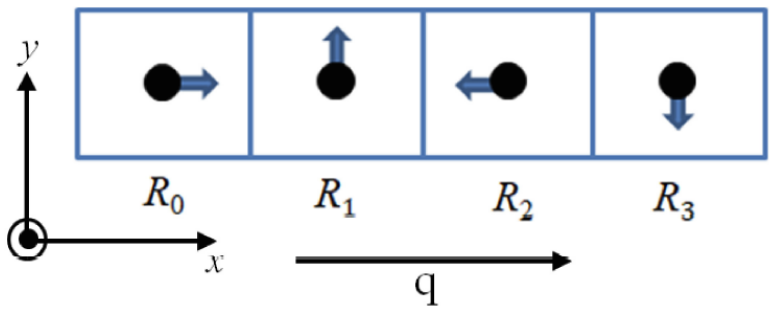
Spin textures for the Rashba spin splitting around gamma-point at the Au(111) surface.



http://www.openmx-square.org/tech_notes/note_kSpin-1_0.pdf

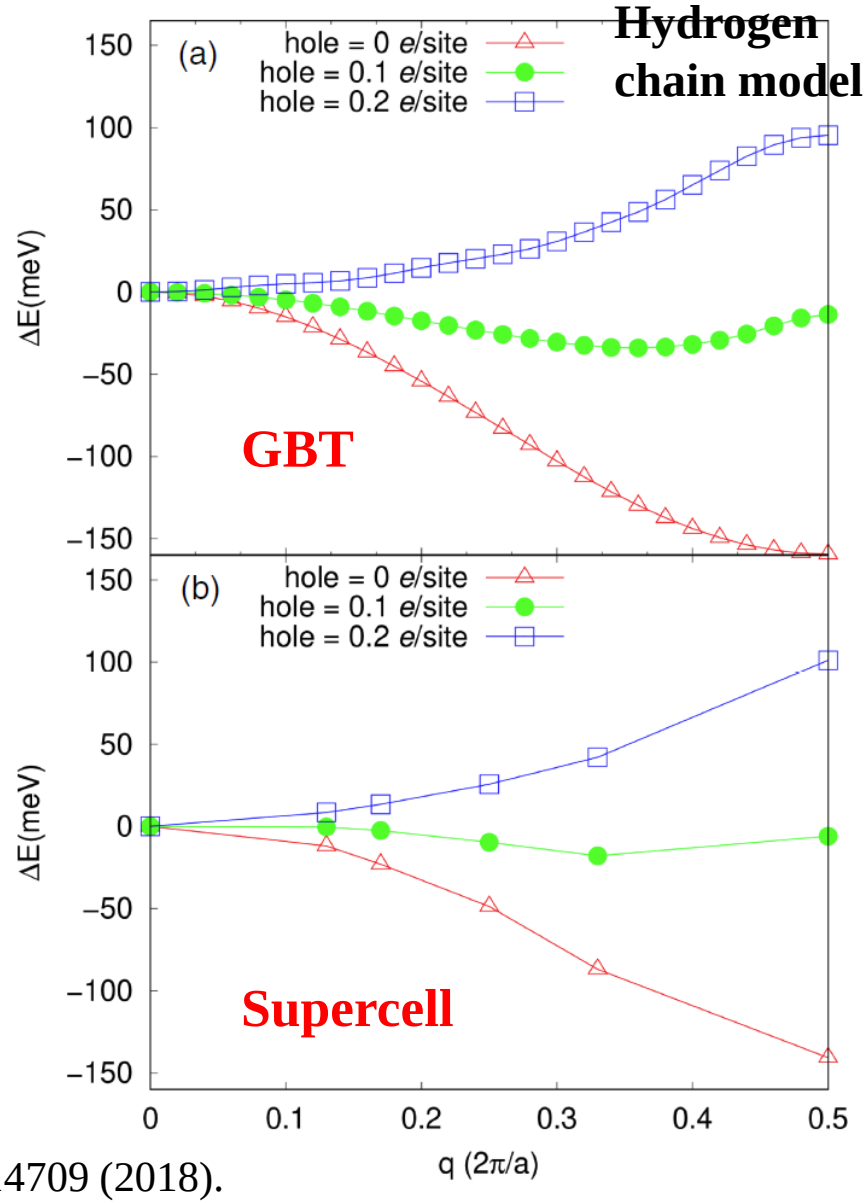
Generalized Bloch theorem for spin spiral supported by Prayitno and Ishii

Spin spiral calculations are supported for the non-collinear DFT without spin orbit coupling (SOC), which is based on the generalized Bloch theorem.



Generalized Bloch theorem (GBT)

$$\psi_{\nu k}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{n}^{N} \sum_{i\alpha} \left[e^{i(k-\frac{q}{2})\cdot \boldsymbol{R}_n} C^{\uparrow}_{\nu k, i\alpha} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + e^{i(k+\frac{q}{2})\cdot \boldsymbol{R}_n} C^{\downarrow}_{\nu k, i\alpha} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] \times \phi_{i\alpha}(\boldsymbol{r} - \tau_i - \boldsymbol{R}_n).$$

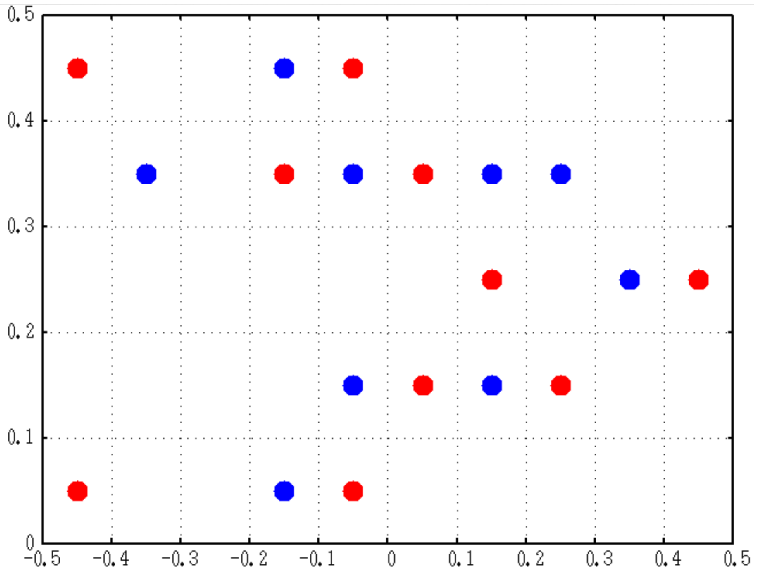


T.B. Prayitno and F. Ishii, J. Phys. Soc. Jpn. **87**, 114709 (2018).

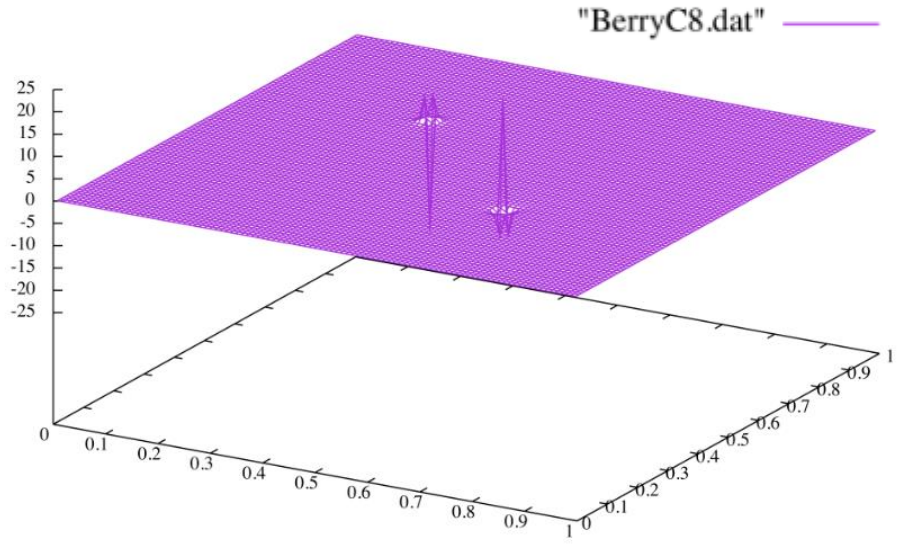
Chern number, Berry curvature, and Z_2 invariant supported by Sawahata and Ishii

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



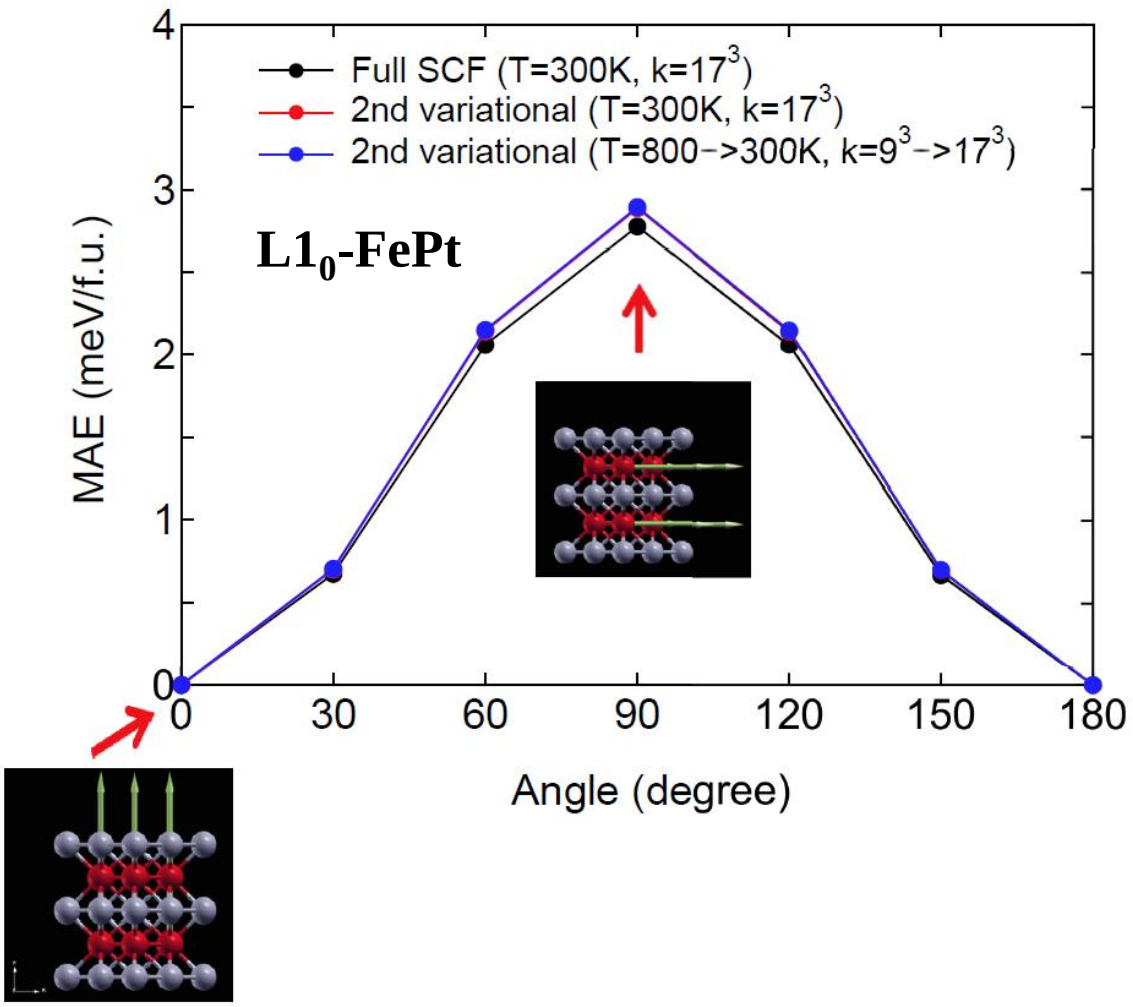
Berry curvature for bands of graphene



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

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).

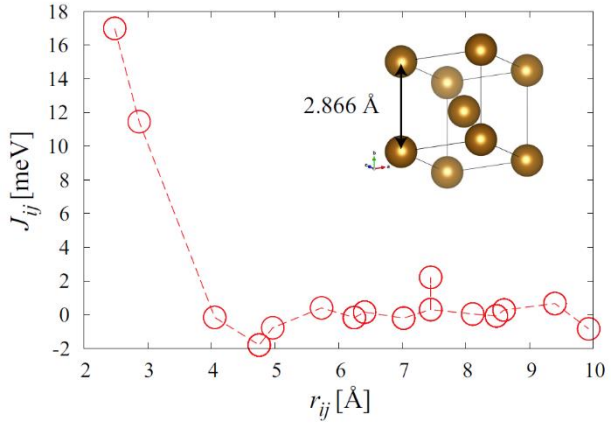


Second variational scheme

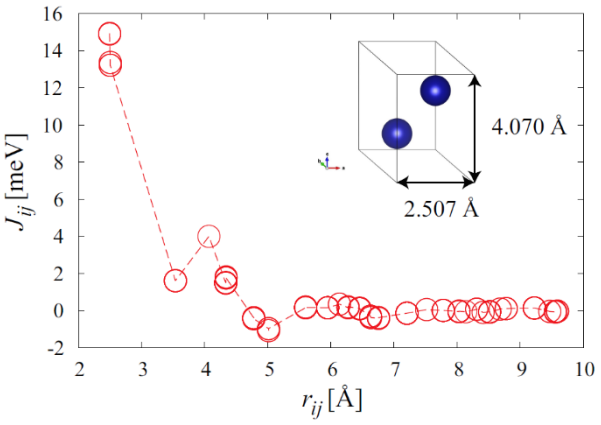
- First, the SCF calculation is performed by the collinear DFT
- Second, with the SCF charge the one-shot diagonalization is performed with SOI.
- The total energy is evaluated by the Harris functional.

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

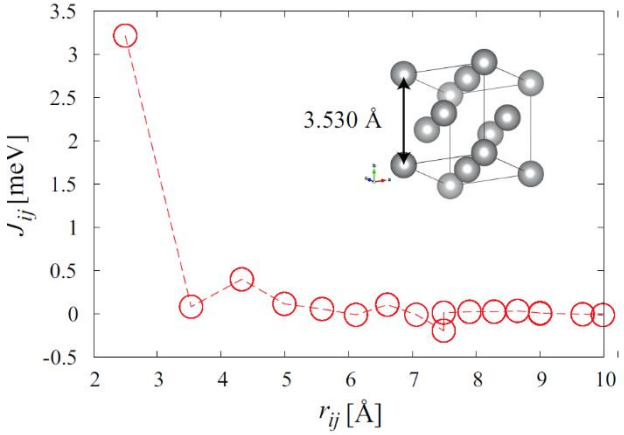
A post-processing code 'jx' to calculate exchange coupling parameters J_{ij} has been largely improved so that the individual J_{ij} in bulks can be calculated efficiently using a contour integration method.



(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	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).

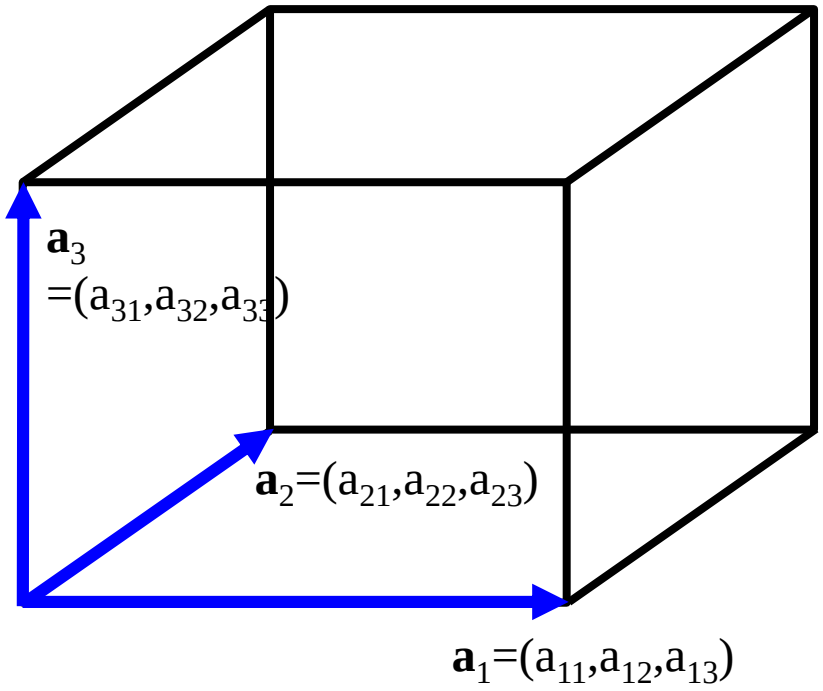
Variable cell optimization with constraints supported by Ozaki

- Variable cell optimization methods with new constraints are supported as 'OptC6', 'OptC7', 'RFC6', and 'RFC7'.

- 'OptC6' is a method that cell vectors and internal coordinates are simultaneously optimized with a constraint that a cell vector $\mathbf{a}_3$ is fixed, while 'OptC7' introduces a constraint that two cell vectors $\mathbf{a}_2$ and $\mathbf{a}_3$ are fixed. In 'OptC6' and 'OptC7' the optimization is performed with a steepest decent method with a variable prefactor.

- 'RFC6' and 'RFC7' behave just like 'OptC6' and 'OptC7', respectively. However, the optimization is performed with the rational function (RF) method.

So, OpenMX Ver. 3.9 supports ten schemes: OptC1, OptC2, OptC3, OptC4, OptC5, OptC6, OptC7, RFC5, RFC6, RFC7



Optimization of enthalpy supported by Ozaki

It is possible to perform the variable cell optimization under an applied pressure, which is done by minimizing the enthalpy.

$$H = E + pV$$

The following output shows how the enthalpy of Si crystal is optimized under a pressure of 10 GPa.

```
************************************************************
                History of cell optimization
************************************************************
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```
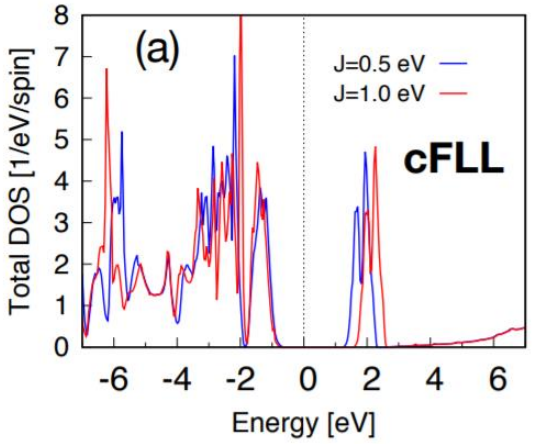
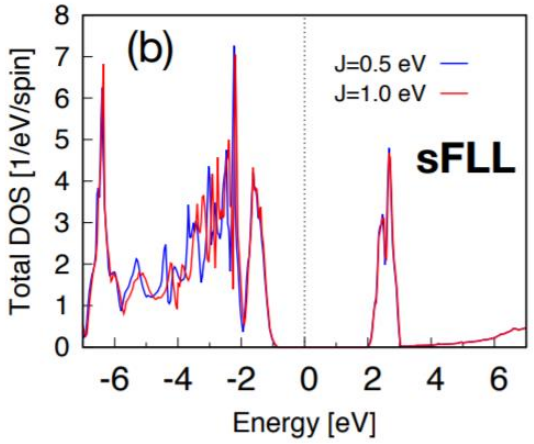

MD_iter	SD_scaling	|Maximum force| (Hartree/Bohr)	Maximum step (Ang)	Utot (Hartree)	Enpy (Hartree)	Volume (Ang^3)
1	1.25981732	0.07663140	0.05108760	-32.84057849	-32.47335956	160.10300700
2	1.25981732	0.06717954	0.04478636	-32.84541333	-32.48138995	158.70978745
3	1.25981732	0.05879663	0.03919775	-32.84853574	-32.48736913	157.46427382
4	1.25981732	0.05131728	0.03421152	-32.85047522	-32.49182806	156.36581813
5	3.14954331	0.04468030	0.07446716	-32.85159836	-32.49515060	155.40690918
6	3.14954331	0.02956430	0.04927383	-32.85232293	-32.50062291	153.33695214
7	3.14954331	0.01960389	0.03267316	-32.85158714	-32.50293764	152.00696345
8	3.14954331	0.01318467	0.02197446	-32.85069024	-32.50392104	151.18717226
9	7.87385828	0.00909382	0.03789092	-32.84998761	-32.50434789	150.69473500
10	7.87385828	0.00253118	0.00537839	-32.84867882	-32.50470324	149.96919000
11	7.87385828	0.00198428	0.03321825	-32.84877730	-32.50477155	149.98234416
12	7.87385828	0.00271856	0.01866538	-32.84922787	-32.50499775	150.08016284
13	7.87385828	0.00086782	0.00943670	-32.84942256	-32.50507226	150.13256385
14	7.87385828	0.00077020	0.00982293	-32.84949585	-32.50509162	150.15607426
15	7.87385828	0.00020223	0.00270074	-32.84950610	-32.50511244	150.15146767
16	7.87385828	0.00005544	0.00000000	-32.84950546	-32.50511390	150.15055140

Generalized DFT+*U* functionals supported by Ryee and Han

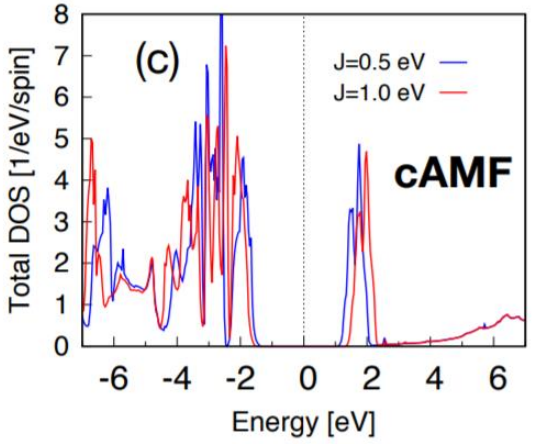
In addition to the simplified rotationally invariant form supported by OpenMX Ver. 3.8, general forms of the DFT+*U* methods are supported with respect to the occupation number operator, the functional form, and the choice of the double counting term for both the collinear and noncollinear calculations.

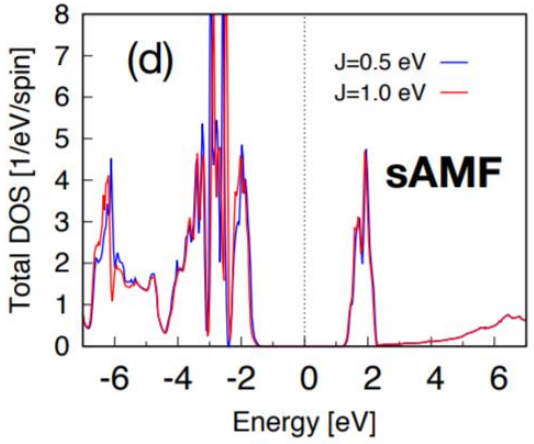




FLL:
fully localized limit

AMF:
around mean-field (AMF)



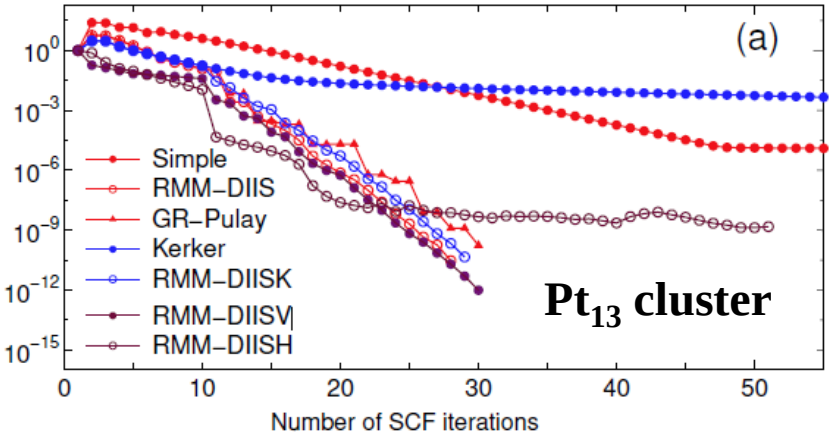


S. Ryee and M.J. Han,
J. Phys:Condens. Matter 30, 275802 (2018).

S. Ryee and M.J. Han,
Scientific Reports 8, 9559 (2018).

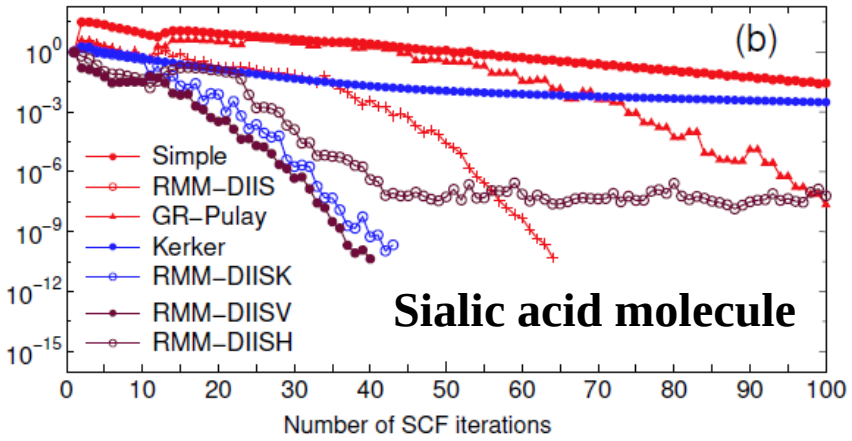
RMM-DIIS mixing for Kohn-Sham potential supported by Ozaki

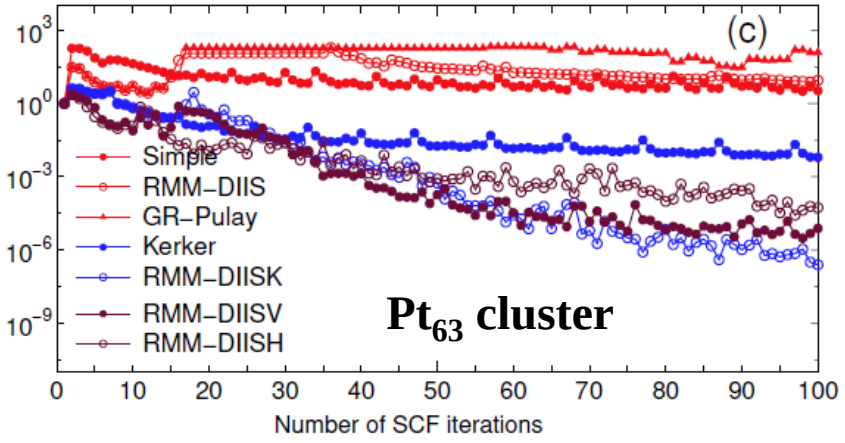
A residual minimization method in the direct inversion iterative subspace (RMM-DIISV) for the Kohn-Sham potentials is supported for the SCF calculations.



For Kohn-Sham potential, the RMM-DIIS mixing method is applied, which is called 'RMM-DIISV'.

It seems that the RMM-DIISV is comparable to RMM-DIISK, and for some cases it outperforms RMM-DIISK.





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).

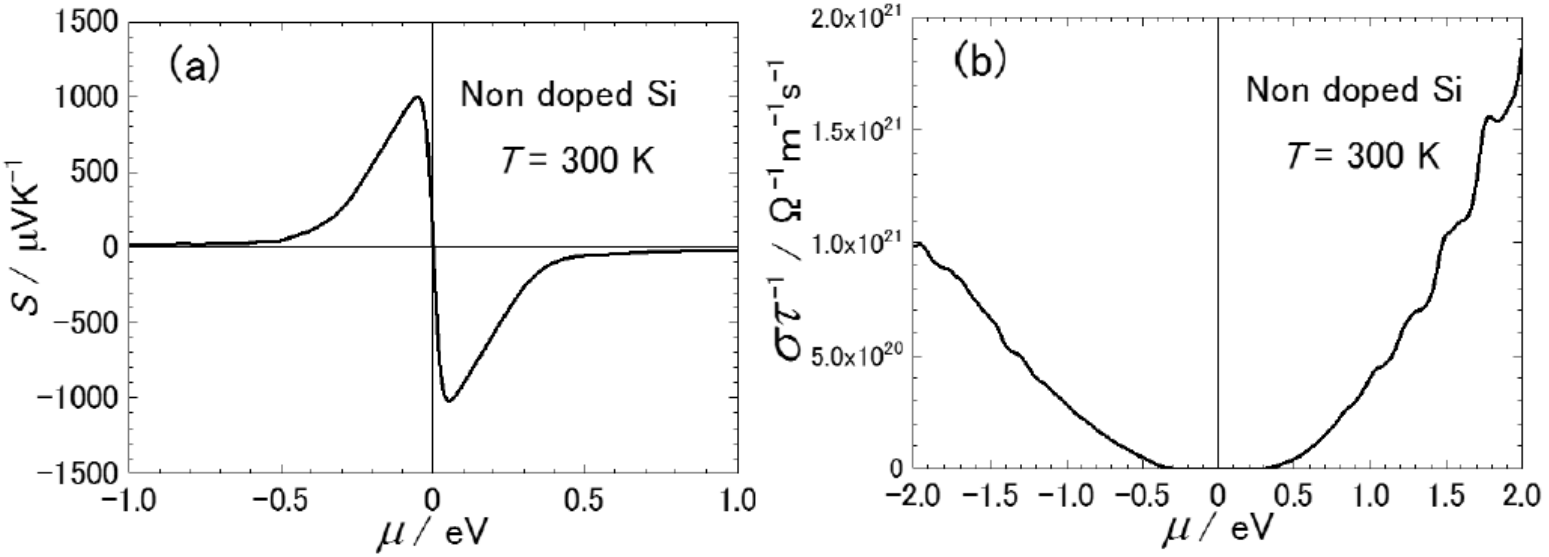


Figure 78: (a) Seebeck coefficient S, and (b) the electric conductivity $\sigma\tau_{\mathrm{el}}^{-1}$ of non-doped Si in the diamond structure as a function of the chemical potential at 300 K obtained by OpenMX and BoltzTraP. The Fourier interpolation factor was set to 25. The input file 'Si_BoltzTraP.dat'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

Calling OpenMX as library or computational engine supported by Ozaki

OpenMX can be utilized as library or computational engine from your program using MPI_Comm_spawn. You may mpirun your program and may want to call OpenMX with different input files from the program in different MPI groups at the same time. In such cases the functionality may be useful.

The following is how to call OpenMX from your code.

```
/* MPI_Comm_spawn */

char command[] = "./openmx";
char **argvin;
char *inputfiles[] = { "Methane.dat", "C60.dat", "Fe2.dat" };

argvin=(char **)malloc(2 * sizeof(char *));
argvin[0] = inputfiles[myworld1];
argvin[1] = NULL;

MPI_Comm_spawn( command, argvin, numprocs1, MPI_INFO_NULL, 0,
                MPI_CommWD[myworld1], &intercomm[myworld1], MPI_ERRCODES_IGNORE );
```

Linkage to other tools #1

- **Trial use**

Some of you might want the quick trial use of OpenMX. The following is one of such tools.
- MateriApps LIVE!:

http://ma.cms-initiative.jp/en/whats-materiapps/try apps/about-materiapps-live?set language=e
MateriApps LIVE! offers an environment where one can try out computational materials science simulation freely, using a notebook PC, etc. All environment required to begin tutorials, such as MateriApps applications, OS (Debian GNU/Linux), editors, and visualization tools, is provided in a USB memory stick. Since OpenMX is available as one of simulation tools in MateriApps LIVE!, you might be able to consider MateriApps LIVE! as an environment for the trial use of OpenMX.

- **Binary distribution**

The binary distribution of OpenMX on LINUX environments is available as follows:

- Debian: https://packages.debian.org/search?keywords=openmx
- Ubuntu: https://launchpad.net/ubuntu/+source/openmx

- **Graphical User Interface (GUI) and/or job scheduling environment**

A couple of GUIs and job scheduling environments for OpenMX calculations are available as follows:

- ASE: https://wiki.fysik.dtu.dk/ase/ase/calculators/openmx.html
- sisl: http://zerothi.github.io/sisl/docs/latest/api-generated/sisl.io.html
- OMXTool: https://github.com/Ncmexp2717/OMXTool
- Winmostar: https://winmostar.com/jp/manual jp/V9/html/winmos/solid/winmos openmx.html

Linkage to other tools #2

- **Visualization in general**

  OpenMX generates cube, md, xyz, xsf, axsf, and cif files. These files can be visualized by many software. The following is some of them.
  - OpenMX Viewer: http://www.openmx-square.org/viewer/
  - XCrySDen: http://www.xcrysden.org/
  - VESTA: http://jp-minerals.org/vesta/en/
  - Molekel: http://www.cscs.ch/molekel/

- **Visualization of Fermi surfaces**

  The Fermi surfaces can be visualized by FermiSurfer.
  - FermiSurfer: http://fermisurfer.osdn.jp/

- **Analysis of molecular dynamics simulations**

  You might want to analyze the trajectory generated by molecular dynamics simulations in OpenMX. The following is one of such tools.
  - ASAP: http://www.mch.rwth-aachen.de/

- **A tool to read and operate OpenMX Kohn-Sham Hamiltonian**

  A tool by Dr. Artem Pulkin is available to read and operate OpenMX Kohn-Sham Hamiltonian at the following website:
  - openmx-hks: https://github.com/pulkin/openmx-hks

Linkage to other tools #3

- **Tight Binding Studio**

  Software package to construct Tight Binding (TB) model in combination with first-principles calculations including the OpenMX code.

  - Tight Binding Studio: https://tight-binding.com/

- **Thermoelectric properties**

  Thermoelectric properties can be calculated by BoltzTraP via an interface with OpenMX or an external tool: QTWARE based on an NEGF method.

  - BoltzTraP: https://doi.org/10.1016/j.cpc.2006.03.007
  - QTWARE: http://www.rs.tus.ac.jp/takahiro/QTWare.html

- **Jx**

  An open source software for calculating magnetic interactions based on magnetic force theory, which is interfaced with OpenMX code. Though the original OpenMX code also supports a similar calculation, the Jx code is a post processing code which has been developed by the Prof. M.J. Han group in KAIST, and released independently.

  - Jx: https://doi.org/10.1016/j.cpc.2019.106927

Linkage to other tools #4

- **Wannier90**

  Maximally localized Wannier functions can be utilized to efficiently and accurately calculate a wide variety of physical properties. OpenMX provides an interface with an post processing code: Wannier90.

  - Wannier90: http://wannier.org/

- **Phonon related properties**

  To calculate phonon related properties such as phonon dispersion and thermal conductivity, OpenMX can be combined with ALAMODE as explained in the following website:

  - ALAMODE: https://alamode.readthedocs.io/en/latest/tutorial.html

- **DCore: DMFT solver interfaced with DFT codes**

  DCore based on dynamical mean-field theory (DMFT) has an interfaces with OpenMX as explained in the following website:

- DCore: https://issp-center-dev.github.io/DCore/master/tutorial/srvo3_openmx/openmx.html#

The other features

The other new features in OpenMX Ver. 3.9 are listed below:

- Requirement of ScaLAPACK and BLACS supported by Ozaki
- Calculations of work functions supported by Yamaguchi and Ozaki
- Improvement of polB supported by Yamaguchi
- Change of the data format for the scfout file supported by Yamaguchi and Ozaki
- Choice of the axis to be treated by ESM method supported by Otani
- A set of choices for the PAO basis functions supported by Ozaki
- ELPA1 and ELPA2 supported by Duy and Ozaki
- Memory reduction for the cluster and band calculations supported by Ozaki
- Interface with FermiSurfer supported by M. Kawamura

Please take a look at the following website for the further details:
http://www.openmx-square.org/whatsnew/whatsnew.html