物質科学のための計算数理 II
Numerical Analysis for Material Science II

8th: Density Functional Theory (1)
Nov. 30 (Fri)

Lecturer: Mitsuaki Kawamura (河村光晶)

Schedule (This semester W1, W2)

1. Sep. 28 (Fri) Guidance Y
2. Oct. 5 (Fri) Monte Carlo method O
3. Oct. 12 (Fri) Monte Carlo method O
4. Oct. 19 (Fri) Monte Carlo method O
5. Oct. 26 (Fri) Exact diagonalization Y
6. Nov. 2 (Fri) Exact diagonalization Y
7. Nov. 9 (Fri) Molecular dynamics O (1st report problem will be announced.)
8. Nov. 30 (Fri) Standard DFT code K
9. Dec. 7 (Fri) Density functional theory K
10. Dec. 14 (Fri) Density functional theory K
11. Dec. 21 (Fri) Density functional theory K
12. Dec. 25 (Tue) (2nd)Report problem K (遠隔講義室)
13. Jan. 11 (Fri) Density functional theory K

※ Lecturers: Y … Yamaji, K … Kawamura, O… Ohgoe

Schedule in this section (DFT)

1. Nov. 30 (Fri) Standard DFT code
   - First-principles calculation and Density functional theory (Lecture)
   - One-body Schrödinger eq. for periodic system and Bloch theorem (L)
   - Numerical solution of Kohn-Sham (one-body Schrödinger) eq. (L)
   - Hands-on DFT code (Tutorial)
   - Version control system : Git (T)
2. Dec. 7 (Fri) Kohn-Sham eq.
   - Plane-wave basis and Pseudopotentials (L)
   - Iterative eigenvalue solution method (L & T)
3. Dec. 14 (Fri) Self-Consistent loop
   - Hartree potential (Poisson eq.)
   - Brillouin-zone integral (Tetrahedron method)
   - Visualization (T)
4. Dec. 21 (Fri) Total Energy
   - Coulomb potential for periodic point charge (Ewald sum)
5. Dec. 25 (Tue) (2nd)Report problem K (遠隔講義室)
6. Jan. 11 (Fri) Density functional theory K

Today's Schedule

What is the first-principles study
Density functional theory
Kohn-Sham method
Periodic system (Bulk crystal)
Bloch theorem
How to solve Kohn-Sham eq. with computer
DFT code
Git clone
Charge density
Band structure
Fermi surface
Density of states (DOS), Partial DOS

Electrons in materials

$$\left[-\sum_{n=1}^{N}\frac{\boldsymbol{\nabla}_n^2}{2}+\frac{1}{2}\sum_{n,n'=1}^{N}\frac{1}{|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|}+\sum_{n=1}^{N}\sum_{I=1}^{N_{\mathrm{atom}}}\frac{Z_I}{|\boldsymbol{r}_n-\boldsymbol{R}_I|}\right]\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N)=E\Psi(\{\boldsymbol{r}_N\})$$

Single H_2O molecule : $N = 10$
Single C_{60} molecule : $N = 360$
Bulk crystal, liquid, glass, ・・・ :
$N > 10^{24}$

Information of electronic structure
- Charge density
- Magnetic moment
- Superconductivity
- Optical spectrum
- etc.

Both numerically and analytically unsolvable.

Can we obtain a few quantities such as
- Ground-state energy
- Ground-state charge density

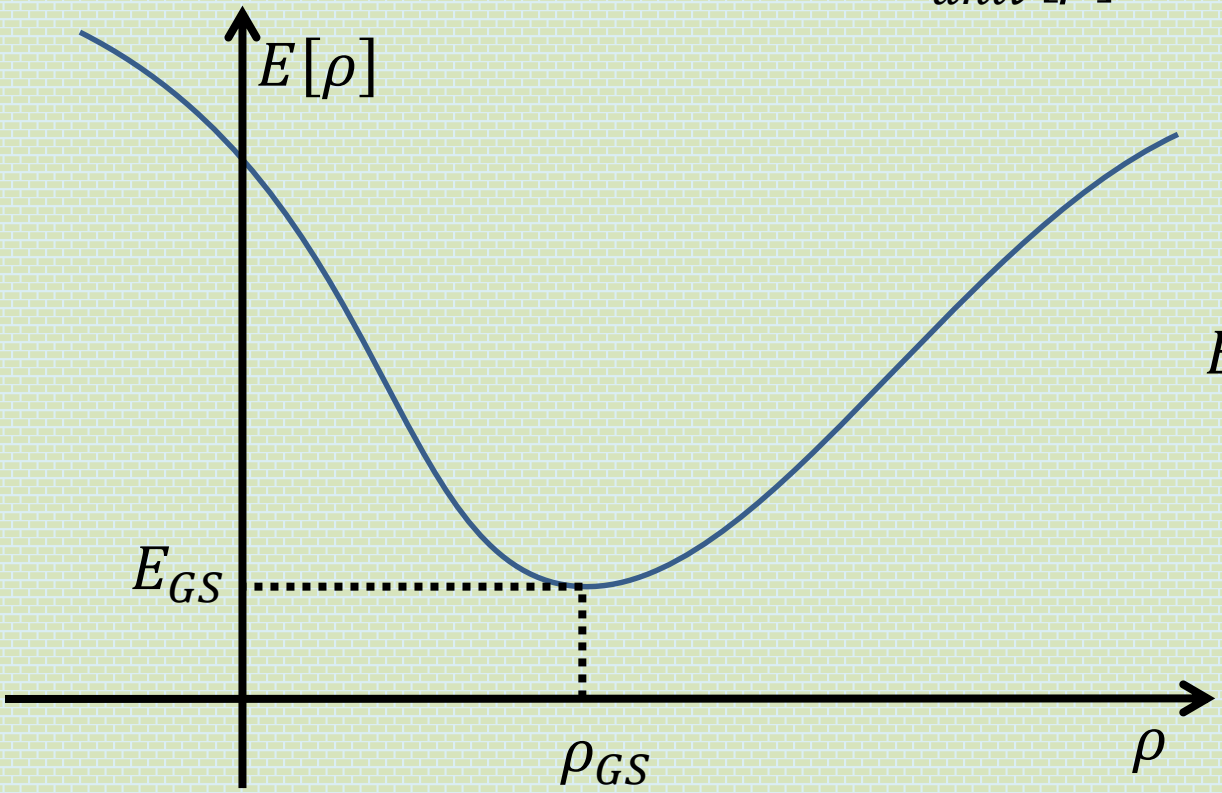
without solving this equation ?

Density functional theory

$$\langle E\rangle = \int d^3r_1 \cdots \int d^3r_N\, \Psi^*(\{\boldsymbol{r}_N\}) \left[-\sum_{n=1}^{N} \frac{\nabla_n^2}{2} + \frac{1}{2} \sum_{n,n'=1}^{N} \frac{1}{|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|} + \sum_{n=1}^{N} v(\boldsymbol{r}_n) \right] \Psi(\{\boldsymbol{r}_N\})$$

$$E[\rho] = \int d^3r \rho(\boldsymbol{r})\, v(\boldsymbol{r}) + E_{univ}[\rho] \qquad v(\boldsymbol{r}) \equiv \sum_{I=1}^{N_{\text{atom}}} \frac{Z_I}{|\boldsymbol{r} - \boldsymbol{R}_I|}$$

Universal functional $E_{univ}[\rho]$ exists.



Functional depends on the overall shape of ρ, e.g.,

$$E_H[\rho] = \frac{1}{2} \iint d^3r d^3r' \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}$$

Hohenberg–Kohn theorem
Phys. Rev. 136, B864 (1964).

Kohn–Sham method

W. Kohn and L. J. Sham,
Phys. Rev. **140**, A1133 (1965).

$$E_{univ}[\rho] = T_{KS}[\rho] + \frac{1}{2}\iint d^3r d^3r' \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + E_{XC}[\rho]$$

Kinetic energy of non–interacting system whose charge density is $\rho(\boldsymbol{r})$

$$\left(-\frac{\boldsymbol{\nabla}^2}{2} + v_{KS}[\rho](\boldsymbol{r})\right)\varphi_n(\boldsymbol{r}) = \varepsilon_n \varphi_n(\boldsymbol{r})$$

$$T_{KS} = 2\sum_{n=1}^{N/2}\int d^3r\, \varphi_n^*(\boldsymbol{r})\left(-\frac{\boldsymbol{\nabla}^2}{2}\right)\varphi_n(\boldsymbol{r})$$

$$\rho(\boldsymbol{r}) = 2\sum_{n=1}^{N/2}|\varphi_n(\boldsymbol{r})|^2$$

$$v_{KS}[\rho](\boldsymbol{r}) = v(\boldsymbol{r}) + \int d^3r' \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + v_{XC}[\rho](\boldsymbol{r})$$

$$v_{XC}[\rho](\boldsymbol{r}) \equiv \frac{\delta E_{XC}[\rho]}{\delta\rho(\boldsymbol{r})}$$

Self–consistent field (SCF)

The exact form of $E_{XC}[\rho]$ is not known.

Approximate $E_{XC}[\rho]$

Local density approximation

$$E_{XC}[\rho] \approx E_{XC}^{LDA}[\rho] \equiv \int d^3r \rho(\boldsymbol{r}) \varepsilon_{XC}\big(\rho(\boldsymbol{r})\big)$$ $\varepsilon_{XC}(\rho)$: Function (not functional)

$$v_{XC}[\rho](\boldsymbol{r}) \approx v_{XC}^{LDA}\big(\rho(\boldsymbol{r})\big) \equiv \frac{\delta E_{XC}^{LDA}[\rho]}{\delta \rho(\boldsymbol{r})} = \varepsilon_{XC}\big(\rho(\boldsymbol{r})\big) + \rho(\boldsymbol{r}) \frac{d\varepsilon_{XC}(\rho)}{d\rho}\Big|_{\rho=\rho(\boldsymbol{r})}$$

$\varepsilon_{XC}(\rho)$: Use the XC energy of homogeneous-electron gas

Random phase approximation : $\varepsilon_{XC}(\rho) = -\frac{0.916}{r_s} + 0.0622 \ln r_s - 0.0938$

M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

$$\frac{4\pi}{3} r_s^3 = \frac{1}{\rho}$$

Monte-Carlo method

$$\varepsilon_{XC}(\rho) = -\frac{0.916}{r_s} + 0.031 \ln r_s - 0.0480 - 0.0116\, r_s + 0.0020 r_s \ln r_s \quad (r_s < 1)$$

[Monte-Carlo] D. M. Ceperley and B.J. Alder, Phys. Rev. Lett. 45, 566 (1980).
[Parameterize] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

$\varepsilon_{XC}(\rho, |\boldsymbol{\nabla}\rho|)$: Generalized gradient correction (GGA)

Total energy and force

$$E_{tot} = \int d^3r_1 \cdots \int d^3r_N \, \Psi^*(\{\boldsymbol{r}_N\}) \left[\sum_{n=1}^{N} \left(\frac{\nabla_n^2}{2} + V(\boldsymbol{r}_n; \{\boldsymbol{R}_{\mathrm{Natom}}\}) \right) + \frac{1}{2} \sum_{n,n'=1}^{N} \frac{1}{|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|} \right] \Psi(\{\boldsymbol{r}_N\})$$

$$+ \frac{1}{2} \sum_{I,J=1}^{N_{\mathrm{atom}}} \frac{Z_I Z_J}{|\boldsymbol{R}_I - \boldsymbol{R}_J|}$$

Nuclear–nuclear interaction

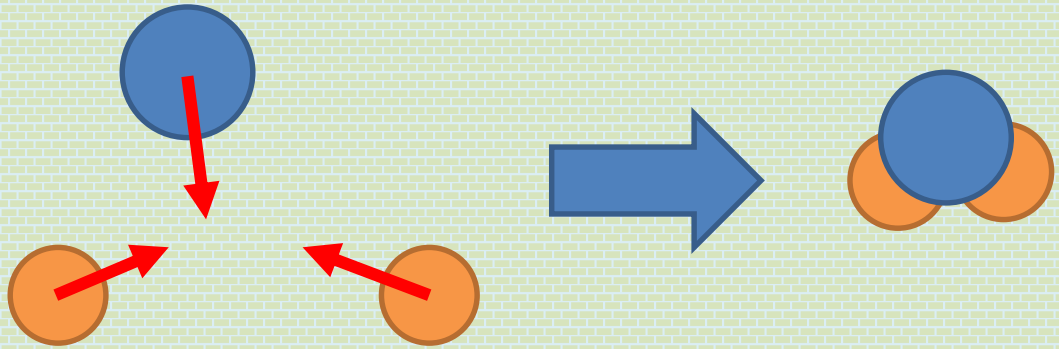
Finding the lowest-energy (stable) structure

Structure optimization : One of the most popular usage of DFT

$$\boldsymbol{F}_I \equiv \frac{\partial E_{tot}}{\partial \boldsymbol{R}_I} = \int d^3r_1 \cdots \int d^3r_N \, \Psi^*(\{\boldsymbol{r}_N\}) \sum_{n=1}^{N} \frac{\partial v(\boldsymbol{r}_n; \{\boldsymbol{R}_{\mathrm{Natom}}\})}{\partial \boldsymbol{R}_I} \Psi(\{\boldsymbol{r}_N\})$$

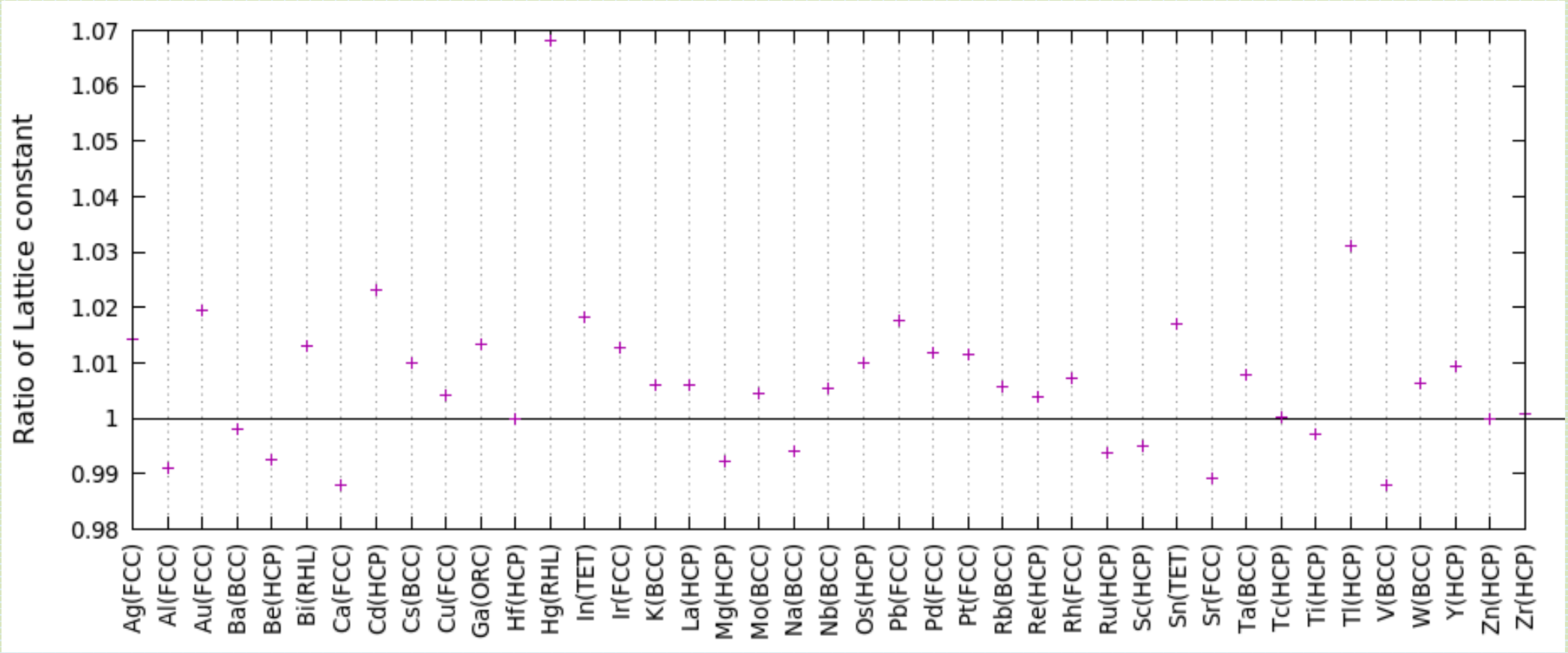
Hellman–Feynmann theorem

$$+ \sum_{J=1}^{N_{\mathrm{atom}}} \frac{Z_I Z_J \, (\boldsymbol{R}_I - \boldsymbol{R}_J)}{|\boldsymbol{R}_I - \boldsymbol{R}_J|^3}$$



Structure optimization

GGA-PBE functional : J. Perdew, K. Burke, and M. Ernzerhof Phys. Rev. Lett. 77, 3865 (1996)



Other usage : Formation (Cohesive) energy

A + B → C + Energy $\quad E_C - (E_A + E_B)$

Magnetic moment (Spin density functional theory) : $E[n_\uparrow, n_\downarrow]$

Kohn–Sham eq. for periodic system (1)

$$\left(-\frac{\nabla^2}{2}+v_{KS}(\boldsymbol{r})\right)\varphi(\boldsymbol{r})=\varepsilon\varphi(\boldsymbol{r})$$

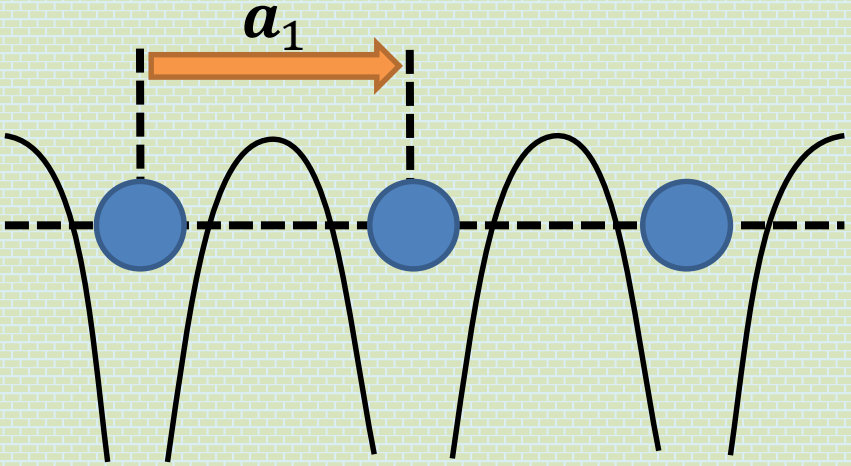
$v_{KS}(\boldsymbol{r})$ and $v(\boldsymbol{r})$ are periodic,
i.e., $v_{KS}(\boldsymbol{r}+n_1\boldsymbol{a}_1+n_2\boldsymbol{a}_2+n_3\boldsymbol{a}_3)=v_{KS}(\boldsymbol{r})$

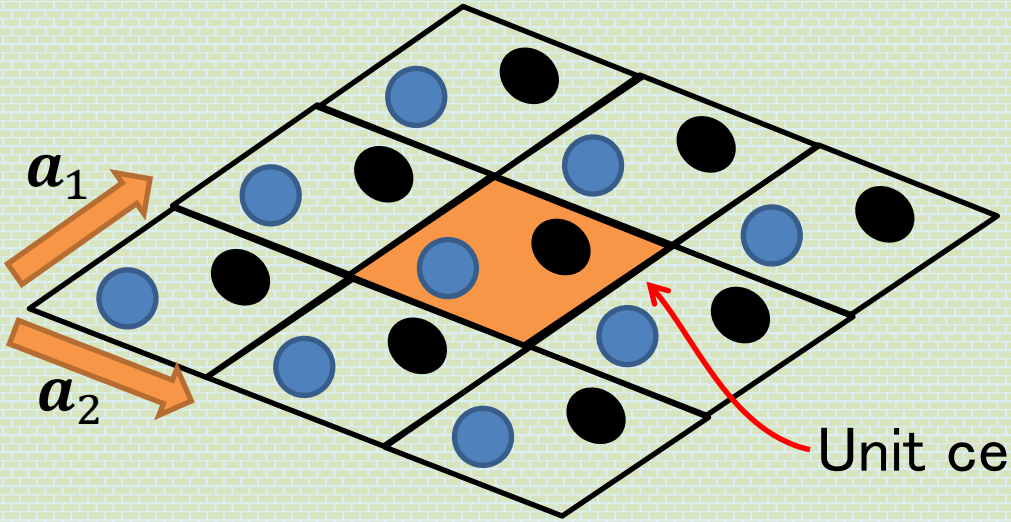
Unit lattice vectors
(Not unique)

$$\rho(\boldsymbol{r})=2\sum_{n=1}^{N\times N_{uc}/2}|\varphi_n(\boldsymbol{r})|^2$$

N electrons per unit cell
N_{uc} cells $\rightarrow \infty$

Equation to solve in the whole region of bulk crystal





Kohn–Sham eq. for periodic system (2)

Bloch's theorem

$\varphi(\boldsymbol{r})$ can be written as

$$\varphi(\boldsymbol{r}) = \frac{1}{\sqrt{N_{uc}}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r} + n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3) = u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$\left(-\frac{(\boldsymbol{\nabla} + \boldsymbol{k})^2}{2} + v_{KS}(\boldsymbol{r})\right) u_{n\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon u_{n\boldsymbol{k}}(\boldsymbol{r})$$

Equation to solve only in the unit cell

$$\int_{uc} d^3r\rho(r) = N$$

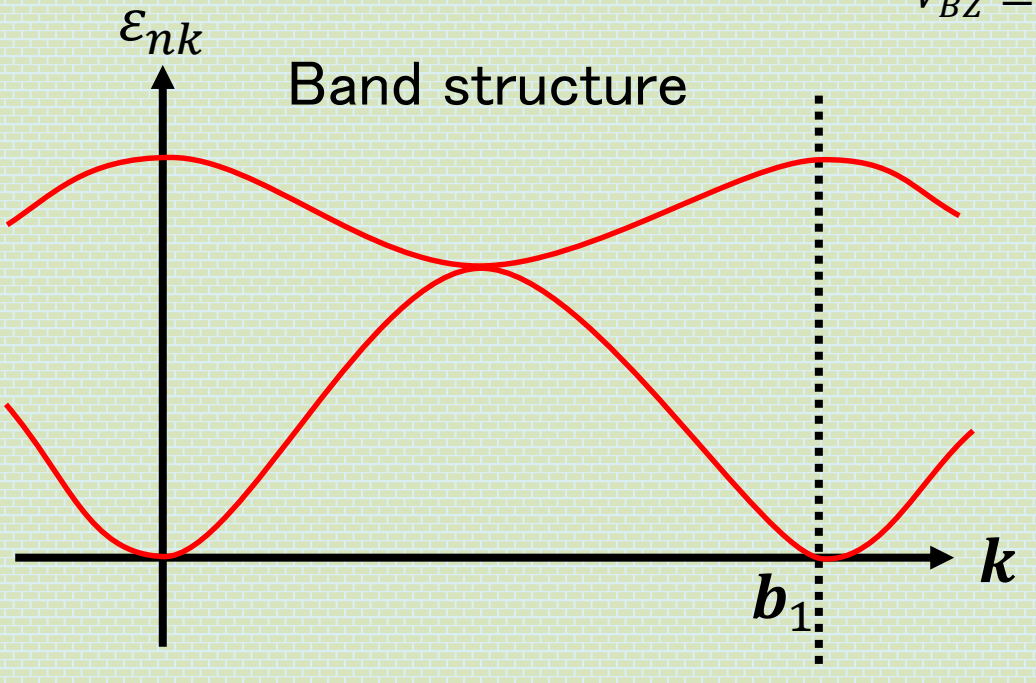
$$\rho(\boldsymbol{r}) = 2\frac{1}{V_{BZ}}\int_{BZ} d^3k \sum_{n=1}^{\infty} |u_{n\boldsymbol{k}}(\boldsymbol{r})|^2\, \theta(\varepsilon_{\mathrm{F}} - \varepsilon_{nk})$$

$$V_{BZ} \equiv \frac{(2\pi)^3}{V_{uc}}$$

$$\begin{pmatrix}\boldsymbol{a}_1\\ \boldsymbol{a}_2\\ \boldsymbol{a}_3\end{pmatrix}(\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3) = 2\pi\hat{I}$$

Unit reciprocal lattice vectors

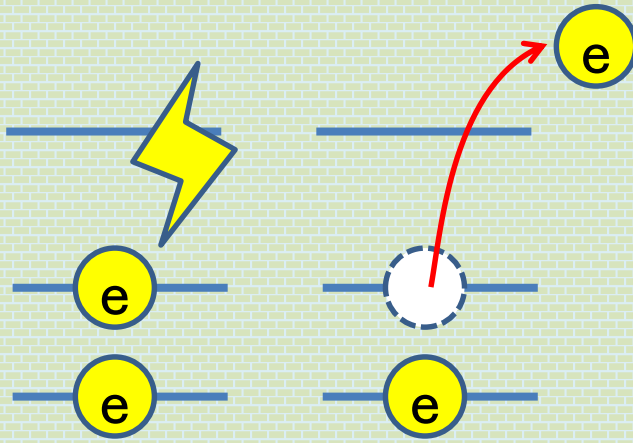
ε_{nk} and $u_{n\boldsymbol{k}}(\boldsymbol{r})$ is periodic with $\boldsymbol{b}_\alpha$ in the $\boldsymbol{k}$ space.



One-body energy level

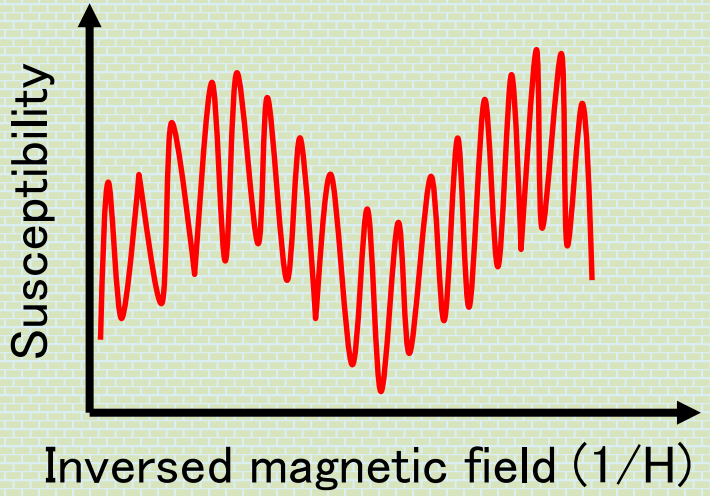
$$\left(-\frac{(\boldsymbol{\nabla}+i\boldsymbol{k})^2}{2}+v_{KS}(\boldsymbol{r})\right)u_{n\boldsymbol{k}}(\boldsymbol{r})=\varepsilon_{nk}u_{n\boldsymbol{k}}(\boldsymbol{r})$$

ε_{nk} ≠True quasi-particle energy

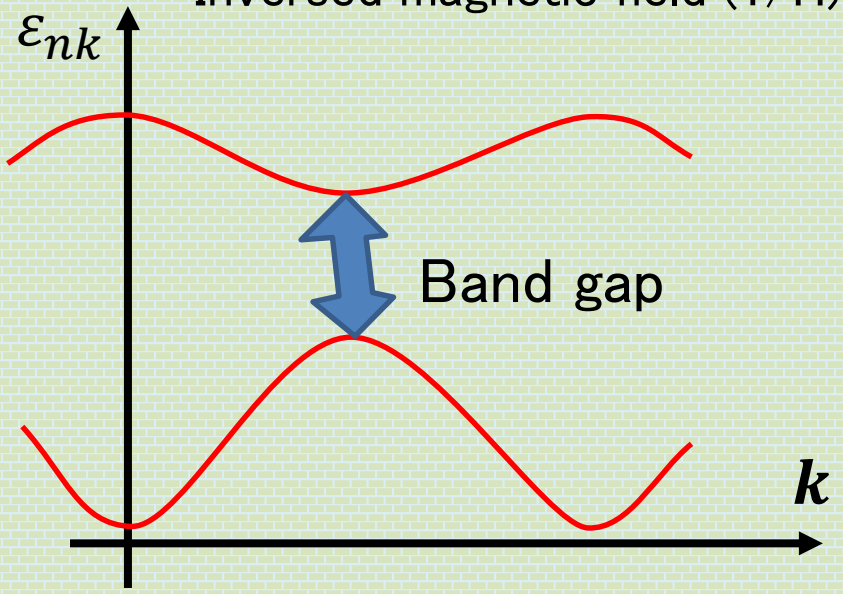


Qualitative analyzation

- Angle resolved photo electronic spectroscopy
- de Haas-van Alphen oscillation



Unit [eV]	LDA	GW	Exp.
Si	0.54	1.32	1.17
LiCl	6.07	9.34	9.40
AlP	1.52	2.59	2.50
AlAs	1.25	2.15	2.23
AlSb	0.99	1.64	1.68
GaP	1.82	2.55	2.39
GaAs	0.37	1.22	1.52
InP	0.57	1.44	1.42



X. Zhu and S. Louie, Phys. Rev. B **43**, 14142 (1991).

How to solve Kohn–Sham eq. : Basis

$$\left(-\frac{(\boldsymbol{\nabla}+i\boldsymbol{k})^2}{2}+v_{KS}(\boldsymbol{r})\right)u_{n\boldsymbol{k}}(\boldsymbol{r})=\varepsilon u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r})\rightarrow u_{n\boldsymbol{k}}(\boldsymbol{r}_i)$$

Huge numerical cost !
Not efficient.

- Pseudopotential (plane wave, real space grid, FEM)
- Local basis (atomic orbital, Gaussian)
- Augmented wave (complicated basis)
- Mixed basis (PW + Local, augmented + Local)

$$u_{n\boldsymbol{k}}(\boldsymbol{r})=\sum_{\alpha}\tilde{u}_{n\boldsymbol{k}\alpha}\,\chi_{\alpha}(\boldsymbol{r})$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r})=\sum_{G}\tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})\frac{e^{i\boldsymbol{G}\cdot\boldsymbol{r}}}{\sqrt{V_{uc}}}$$

$$\left(-\frac{(\boldsymbol{G}+\boldsymbol{k})^2}{2}+\hat{v}_{KS}\right)\tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})=\varepsilon\tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})$$

Plane waves below the
Cutoff frequency

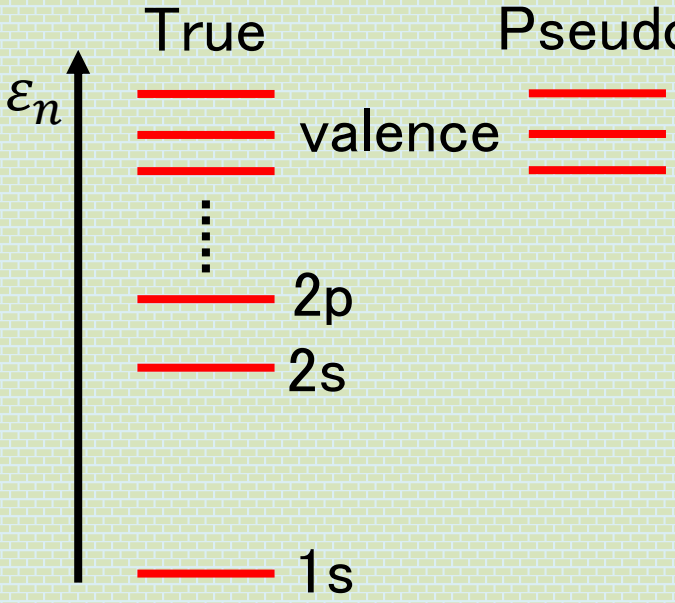
$$\hat{v}_{KS}\tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})=\int_{uc}d^3r\frac{e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}}{\sqrt{V_{uc}}}v_{KS}(\boldsymbol{r})u_{n\boldsymbol{k}}(\boldsymbol{r})$$

Pseudopotential

Electronic state at core level (e.g. 1s state for Fe)

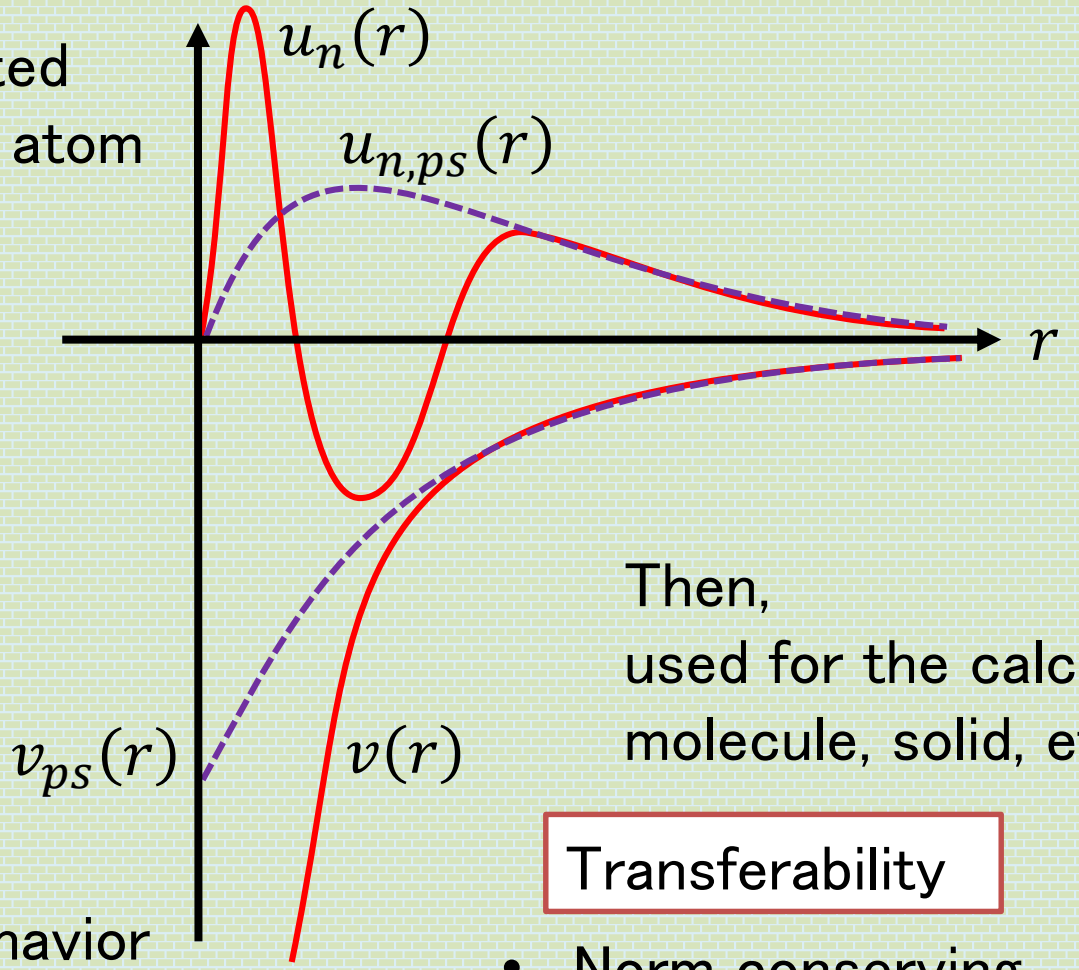
hardly affects the chemical properties
(chemical reaction, conduction, superconductivity, etc.)

Pseudopotential is generated
in the calculation of single atom



only reproduce the
energy and long-range behavior
of valence state.

Similar to the potential of an ion.



Then,
used for the calculation of
molecule, solid, etc.

Transferability

- Norm conserving
- Ultrasoft
- Projector augmented wave

QuantumESPRESSO:

plane wave and pseudopotential based code

Before the explanation, we should start to install because it takes long time.

mac OSX in ECCS

```
$ mkdir -p ~/bin/
$ echo 'export PATH=$HOME/bin:$PATH' >> ~/.profile
$ git clone https://gitlab.com/QEF/q-e.git -b qe-6.3 ~/q-e
$ cd ~/q-e/
$ ./configure CC=gcc-8; make pw pp; cp bin/* ~/bin/
```

Prompt. We do not need type this.

Quantum ESPRESSO

Web page : https://www.quantum-espresso.org/

Developer : P Giannozzi (University of Udine, Italy), *et al.* (Many)

Language : Fortran (Mainly)

Feature:

- Total energy, force, MD, chemical reaction path, charge/spin density
- Band structure, density of states, Fermi surfaces
- LDA, GGA, Van der Waals, exact exchange functional
- MPI+OpenMP parallelism, GPGPU
- Phonon and electron-phonon interaction
- X-ray absorption spectra, Optical spectra
- Many-body perturbation theory (GW, Bethe-Salpeter eq.)
- Wannier function, Berry's phase
- Etc.

Manuals : https://www.quantum-espresso.org/resources/users-manual

Pseudopotential library

- SSSP (https://www.materialscloud.org/discover/sssp/table/efficiency)
- PSLibrary (https://www.quantum-espresso.org/pseudopotentials)

Visualization tools

FermiSurfer : Fermi-surface viewer

```
$ git clone https://scm.osdn.net/gitroot/fermisurfer/fermisurfer.git -b 1.10.1 ~/fermisurfer
$ cd ~/fermisurfer/
$ touch Makefile.in aclocal.m4 configure
$ ./configure --prefix=$HOME; make; make install
```

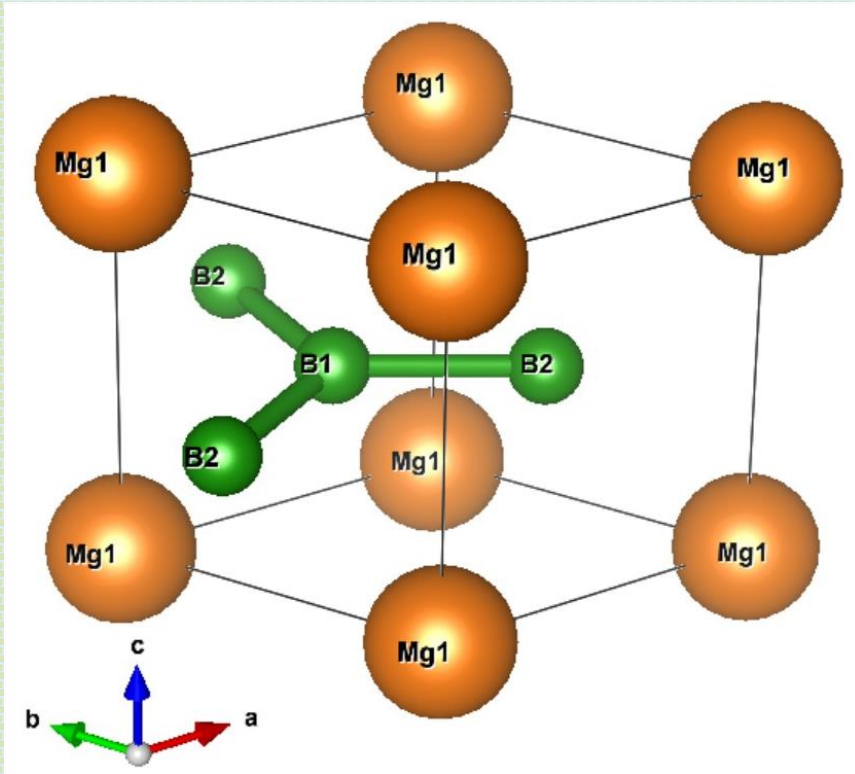
VESTA : Crystal-structure viewer (Also charge density, etc.)

```
$ wget https://jp-minerals.org/vesta/archives/3.4.5/VESTA.dmg
$ hdiutil mount VESTA.dmg
$ cp -rf /Volumes/VESTA/VESTA ~/
$ echo 'alias vesta="open -a $HOME/VESTA/VESTA.app"' >> ~/.profile
$ source ~/.profile
```

Tutorial : MgB_2

```
$ wget https://osdn.net/projects/educational-pwdft/storage/113018.tgz
$ tar xzvf 113018.tgz -C ~/
$ cd ~/113018/
$ vesta mgb2.xsf
```

- Metal
- Superconductivity : T_C = 39 K
- Stacked Mg triangular lattice and B honeycomb lattice



Structure optimization & input file

```
$ mpirun -np 2 ~/bin/pw.x -npool 2 -in relax.in | tee relax.out
```

```
&CONTROL
 calculation = 'vc-relax'
  pseudo_dir = './'
/
&SYSTEM
       ibrav = 0
         nat = 3
        ntyp = 2
     ecutwfc = 35.000000
     ecutrho = 280.000000
 occupations = 'tetrahedra_opt'
/
&ELECTRONS
/
&IONS
/
&CELL
/
```

Variation-cell structure relaxation

Number of atoms in the unit cell

Number of kinds of atom

Cutoff energy of plane-waves for wave functions [Ry]

$$u_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_{G} \tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})\, e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

Cutoff depends on the pseudopotential

Cutoff energy of plane-waves for the charge density [Ry]

Integration scheme for the numerical integration in

$$\rho(\boldsymbol{r}) = 2\frac{1}{V_{BZ}}\int_{BZ} d^3k \sum_{n=1}^{\infty} |u_{n\boldsymbol{k}}(\boldsymbol{r})|^2 \theta(\varepsilon_{\mathrm{F}} - \varepsilon_{n\boldsymbol{k}})$$

Input-file format

```
CELL_PARAMETERS angstrom
   3.200000   0.000000 0.000000
  -1.600000   2.771281 0.000000
   0.000000   0.000000 3.700000
ATOMIC_SPECIES
 B 10.811000 b_pbe_v1.4.uspp.F.UPF
 Mg 24.305000 Mg.pbe-n-kjpaw_psl.0.3.0.UPF
ATOMIC_POSITIONS crystal
 Mg 0.000000 0.000000 0.000000
 B 0.333333 0.666667 0.500000
 B 0.666667 0.333333 0.500000
K_POINTS automatic
 12 12 8 0 0 0
```

Unit lattice vectors (Å unit)

Element

Relative atomic mass

Pseudopotential file name

Atomic position in the fractional coordinate

$$\boldsymbol{R} = x_1\boldsymbol{a}_1 + x_2\boldsymbol{a}_2 + x_3\boldsymbol{a}_3$$

$\boldsymbol{k}$-mesh for numerical integration in

$$\rho(\boldsymbol{r}) = 2\frac{1}{V_{BZ}}\int_{BZ} d^3k \sum_{n=1}^{\infty} |u_{n\boldsymbol{k}}(\boldsymbol{r})|^2\,\theta(\varepsilon_{\mathrm{F}} - \varepsilon_{nk})$$

Dense k-mesh improves accuracy and increases numerical cost.

Result

```
$ grep volume relax.out
relax.out:     unit-cell volume           =     221.4261 (a.u.)^3
relax.out:     new unit-cell volume =    204.22304 a.u.^3 (    30.26273 Ang^3 )
relax.out:     new unit-cell volume =    193.53924 a.u.^3 (    28.67956 Ang^3 )
relax.out:     new unit-cell volume =    194.50016 a.u.^3 (    28.82195 Ang^3 )
relax.out:     new unit-cell volume =    194.38563 a.u.^3 (    28.80498 Ang^3 )
relax.out:     new unit-cell volume =    194.25661 a.u.^3 (    28.78586 Ang^3 )
relax.out:     new unit-cell volume =    194.25661 a.u.^3 (    28.78586 Ang^3 )
relax.out:     unit-cell volume           =     194.2566 (a.u.)^3
$ grep -A 3 CELL_PARAMETERS relax.out
CELL_PARAMETERS (angstrom)
   3.106677678   0.000000000  -0.000000000
  -1.553338839   2.690461490   0.000000000
   0.000000000  -0.000000000   3.620638395
 :
--
CELL_PARAMETERS (angstrom)
   3.072422829   0.000000000   0.000000000
  -1.536211414   2.660795917   0.000000000
   0.000000000   0.000000000   3.521167214
```

Exp. (XRD)

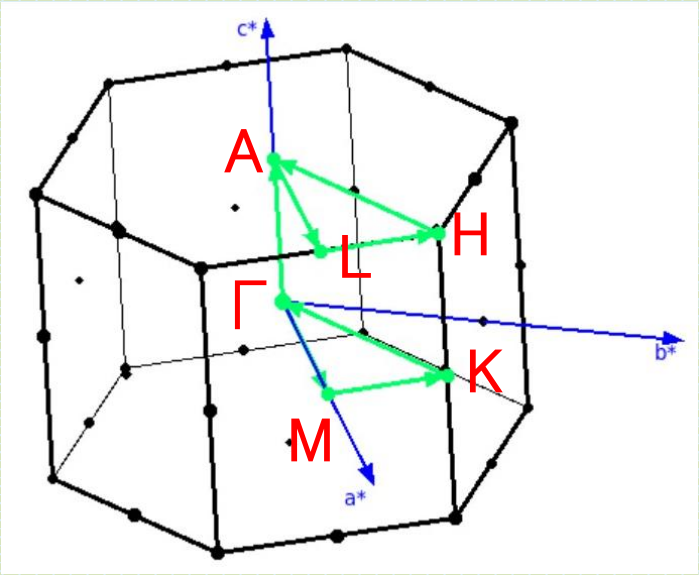
a = 3.085 Å, c = 3.523 Å

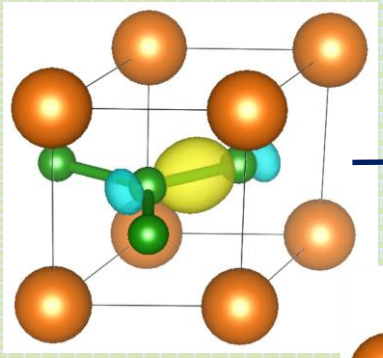
volume : 29.04 $Å^3$

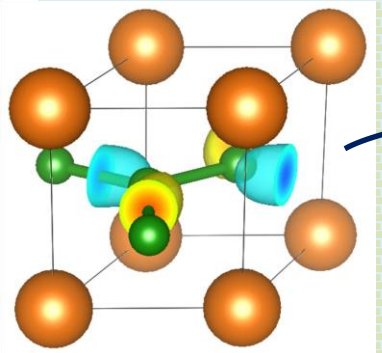
Band structure

```
$ mpirun -np 2 ~/bin/pw.x -npool 2 -in nonscf.in
$ mpirun -np 2 ~/bin/bands.x -npool 2 -in bands.in
$ gnuplot band.gp
```

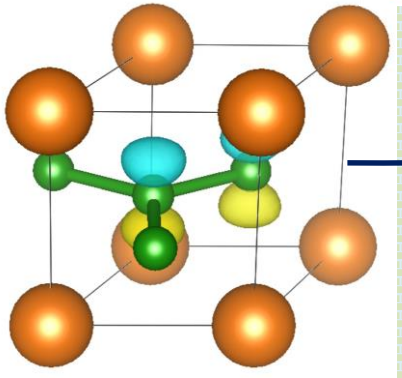
```
$ mpirun -np 1 ~/bin/pp.x -npool 1 -in pp.in
$ vesta tmp.pp_K001_B00*.xsf
```

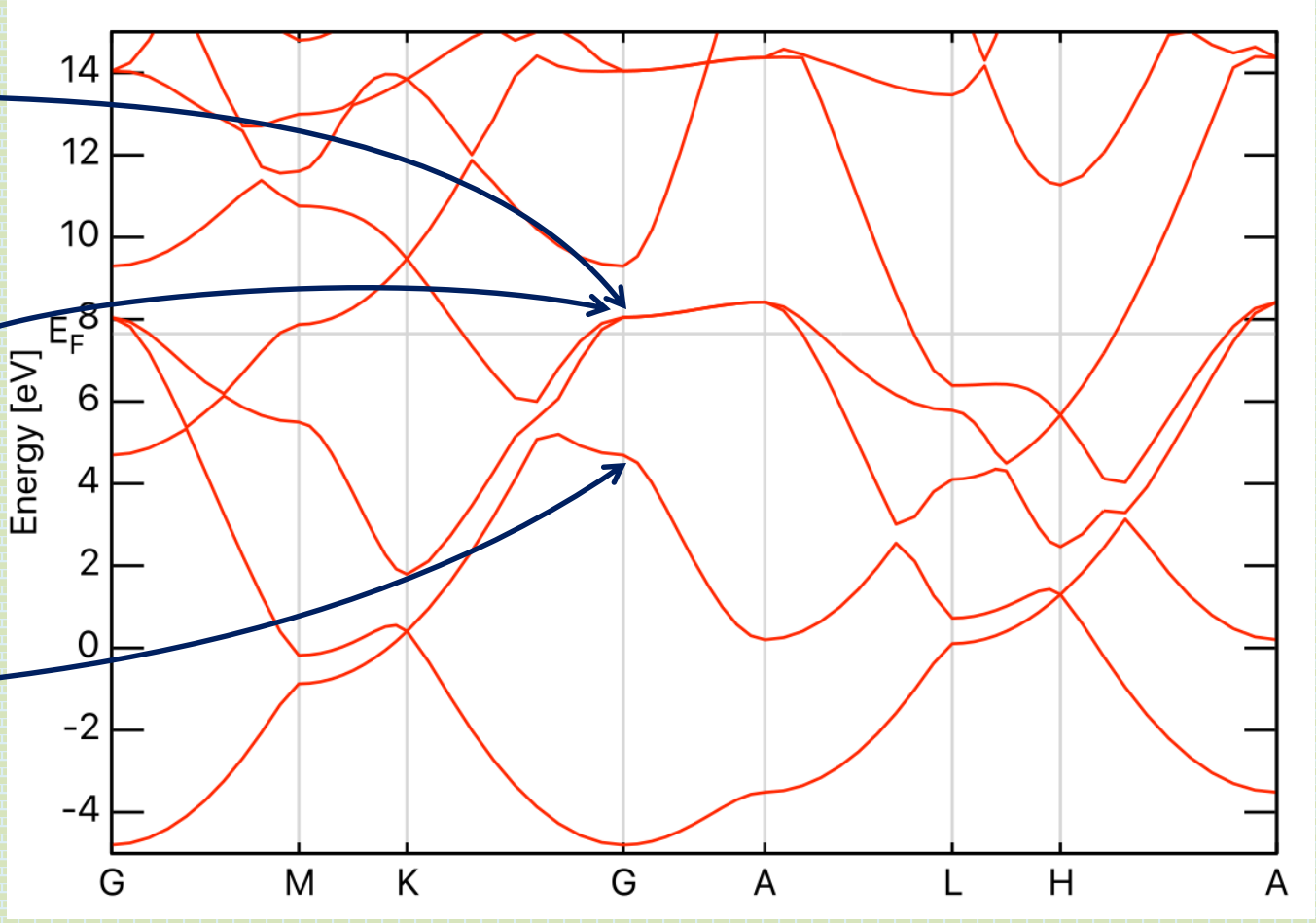






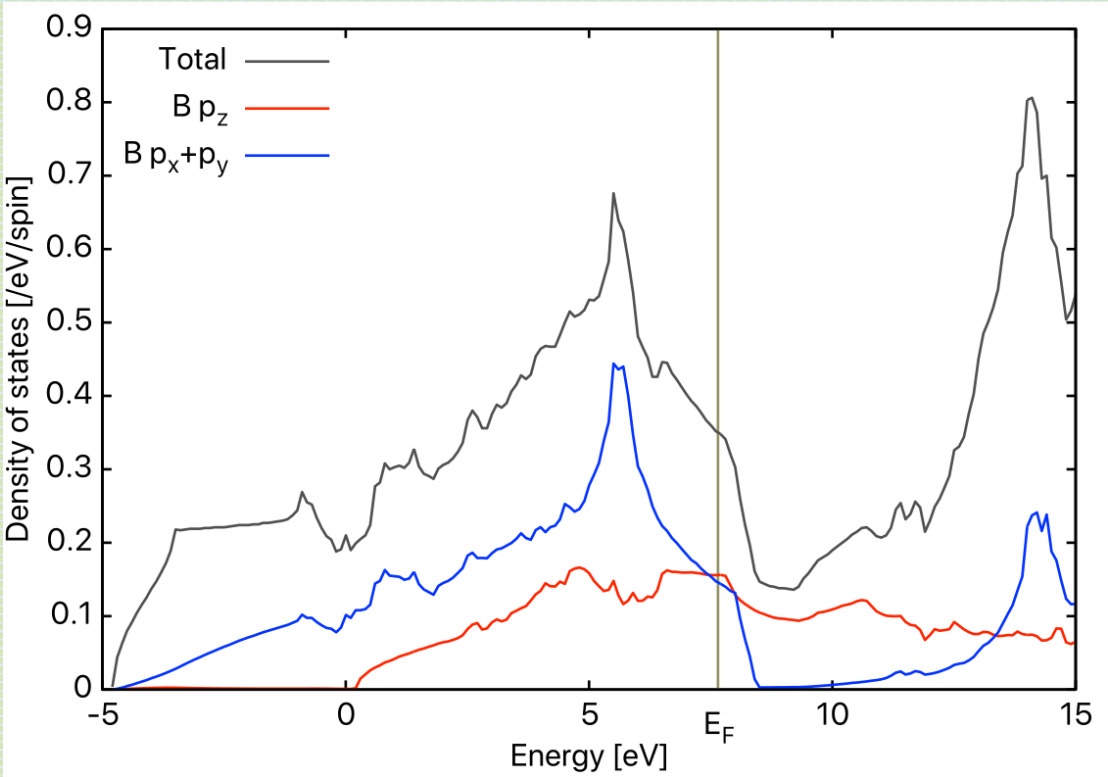
$u_{nk}(\boldsymbol{r})$





Density of states & Fermi surface

```
$ mpirun -np 2 ~/bin/pw.x -npool 2 -in dense.in
$ mpirun -np 2 ~/bin/projwfc.x -npool 2 -in pdos.in |tee pdos.out
$ gnuplot pdos.gp
```

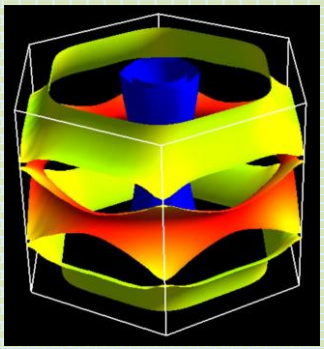


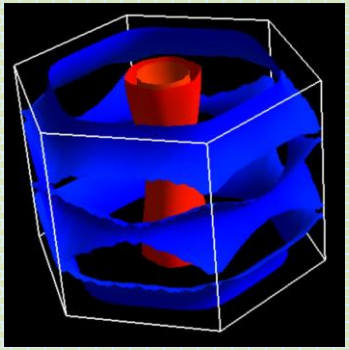
$$D(\varepsilon) = \frac{1}{V_{BZ}} \int_{BZ} d^3k \sum_{n=1}^{\infty} \delta(\varepsilon - \varepsilon_{nk})$$

$$D_p(\varepsilon) = \frac{1}{V_{BZ}} \int_{BZ} d^3k \sum_{n=1}^{\infty} \delta(\varepsilon - \varepsilon_{nk}) \times \left| \int d^3r \psi_p^*(\boldsymbol{r}) \varphi_{nk}(\boldsymbol{r}) \right|^2$$

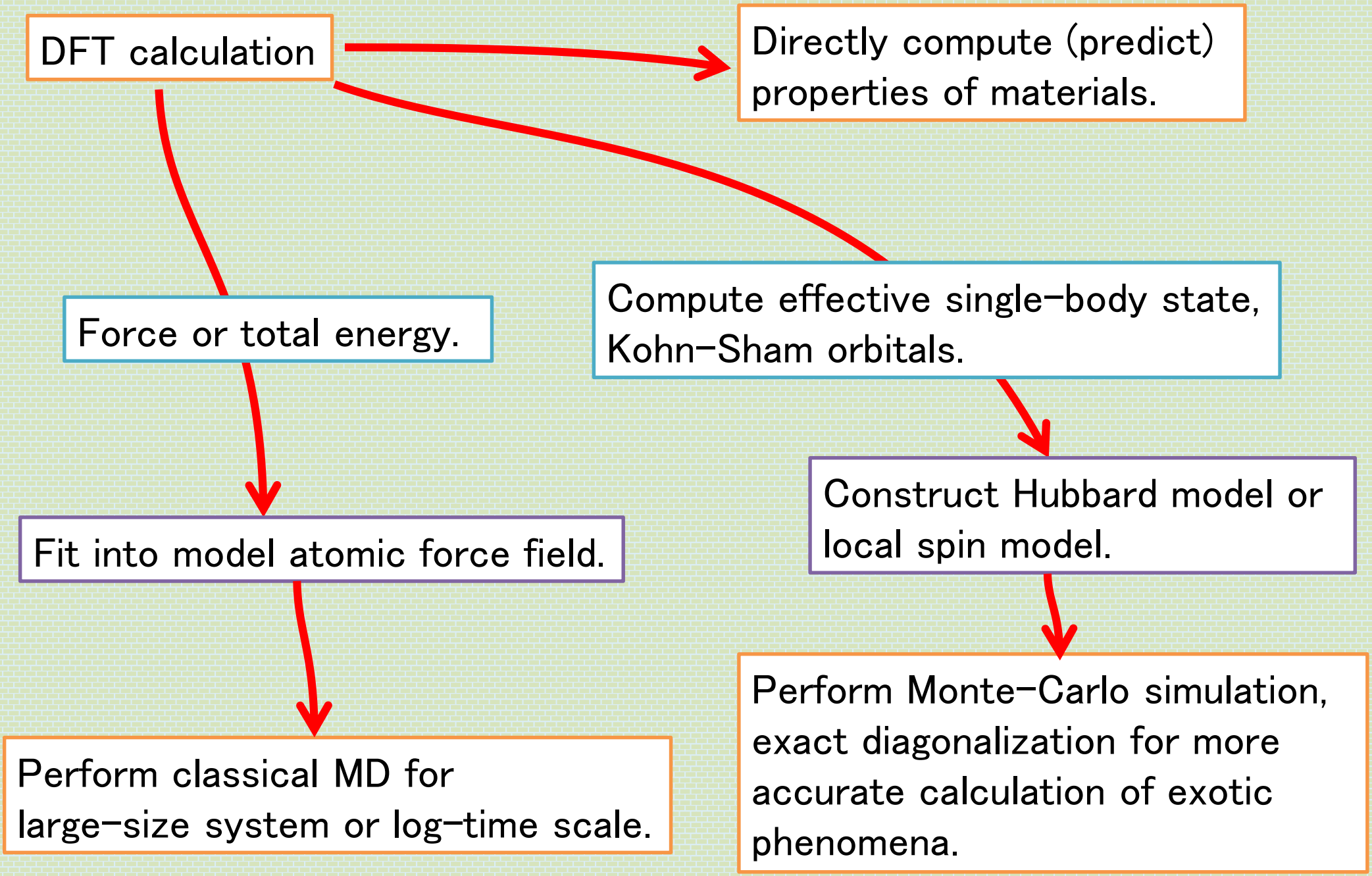
Fermi surface :
Isosurface at $\varepsilon_{nk} = \varepsilon_{\mathrm{F}}$

```
$ mpirun -np 1 ~/bin/fermi_proj.x -in proj_pz.in
$ mv proj.frmsf pz.frmsf
$ mpirun -np 1 ~/bin/fermi_proj.x -in proj_pxy.in
$ mv proj.frmsf pxy.frmsf
$ fermisurfer pz.frmsf
$ fermisurfer pxy.frmsf
```





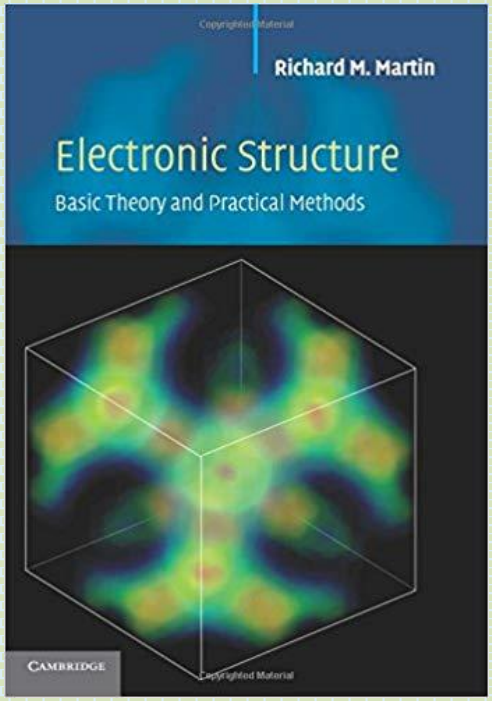
Why do we perform DFT calculation ?



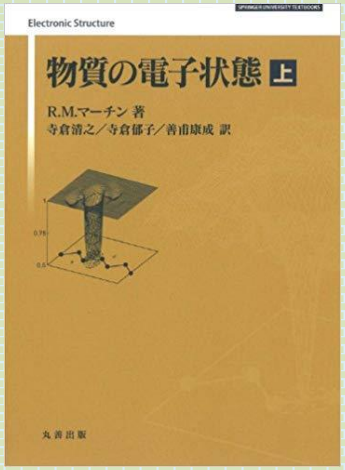
Today's summary

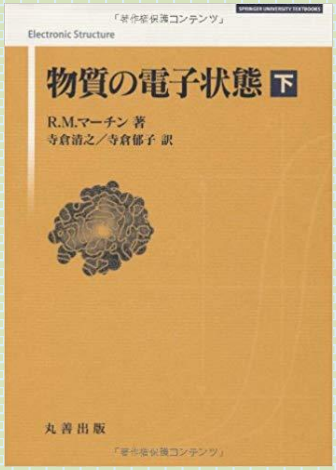
- Basics of DFT calculation
  - Hohenberg–Kohn theorem
  - Kohn–Sham method
  - Exchange correlation functional
  - Total energy and force
- Kohn–Sham eq. in periodic system (bulk crystal)
  - Bloch theorem
  - Band structure
- Numerical method to solve Kohn–Sham eq.
  - Plane-wave (and other) basis
  - Pseudopotential
- Usage of a DFT code : Quantum ESPRESSO

Reference books



Electronic Structure: Basic Theory and Practical Methods
Richard M. Martin
Cambridge University Press
Errata : https://es.polytechnique.fr/Electronic_Structure/errata





日本語訳
物質の電子状態 上下
寺倉清之、寺倉郁子、善甫康成
シュプリンガー

固体-構造と物性
金森 順次郎, 川村 清, 米沢 富美子, 寺倉 清之
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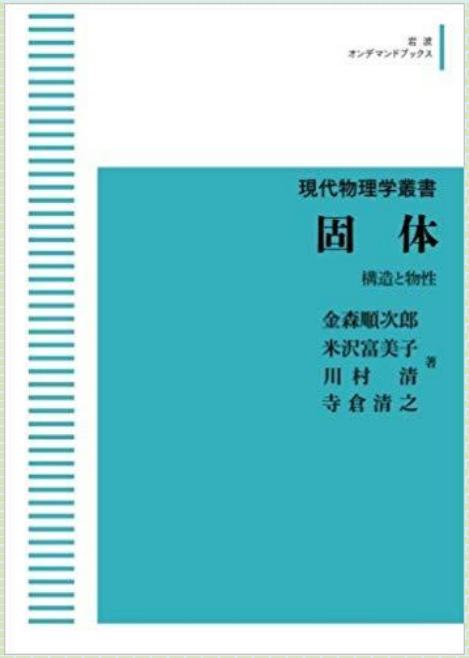

岩波オンデマンド