OSAKA UNIVERSITY

大阪大学
社会人教育プログラム

# FLAPW法の基礎

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HiLAPW

# OUTLINE

- FLAPW Method
  - One-electron equations and Bloch function
  - APW method
  - Linear method
  - Full-potential method
- FLAPW Codes
  - FLAPW packages open to public

# Kohn-Sham Equations

$$\mathcal{H}\psi_j(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{eff}}(\mathbf{r})\right]\psi_j(\mathbf{r}) = \varepsilon_j\psi_j(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_j |\psi_j(\mathbf{r})|^2$$

$$v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + e^2\int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \mu_{\text{xc}}(n(\mathbf{r}))$$

**★ One-electron equations to describe independent Fermi particles in an effective field determined in a self-consistent way.**

# Band Theory

## How to solve the one-electron equations for particular condensed-matter systems

**Periodic system → Band theory**

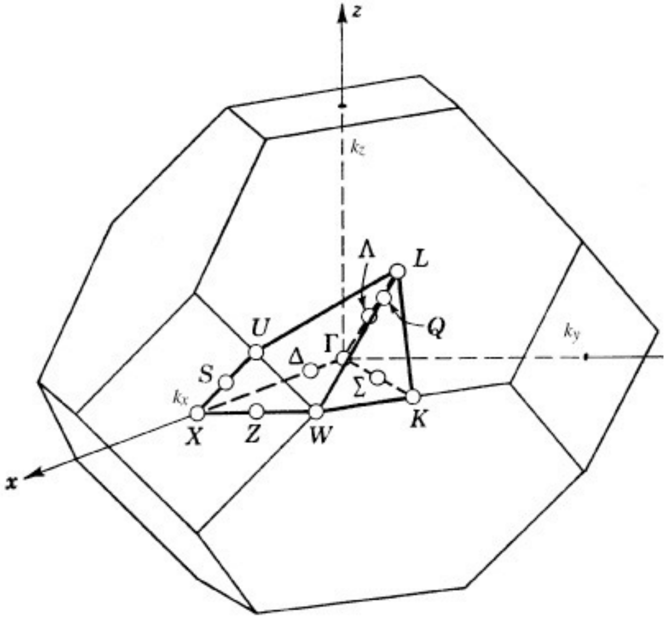
**Bloch Theorem**

**★A quantum-mechanical state in a periodic system can be specified with a wave number k**

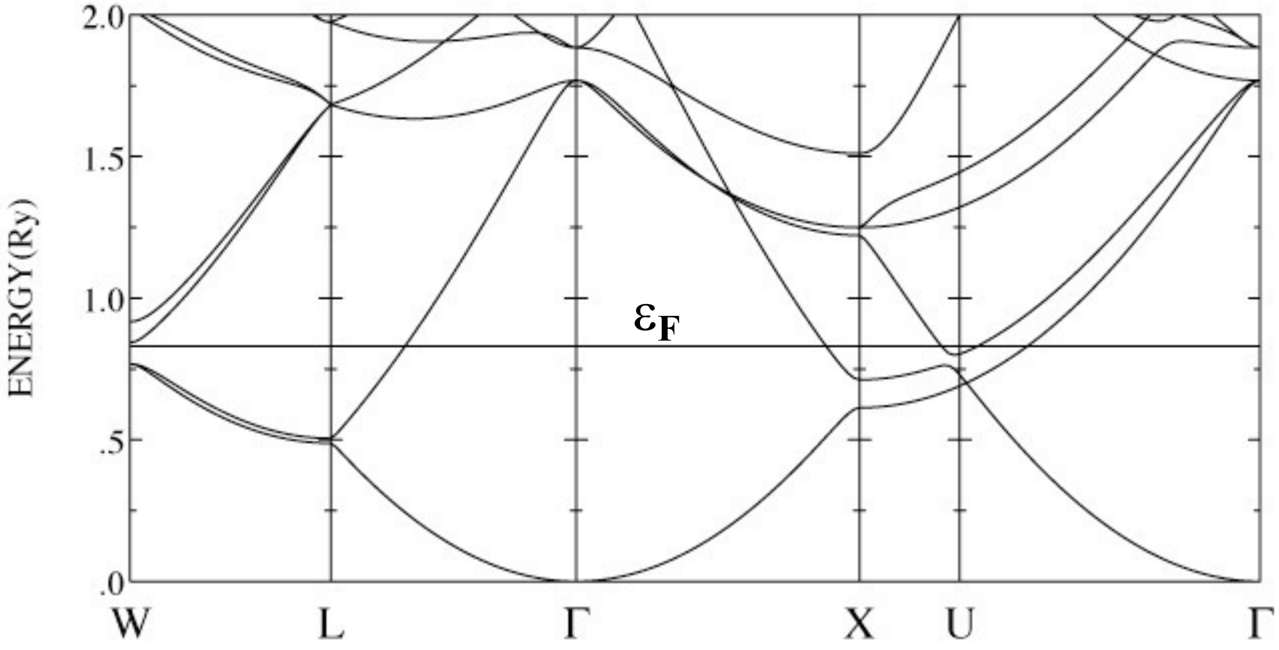
$$\mathcal{H}\psi_j^{\mathbf{k}}(\mathbf{r}) = \boxed{\varepsilon_j^{\mathbf{k}}}\psi_j^{\mathbf{k}}(\mathbf{r})$$

**Dispersion relation: band structure**

# Brillouin Zone and Bands



**BZ of fcc lattice**



**Band structure of fcc Al**

**independent quantum number**

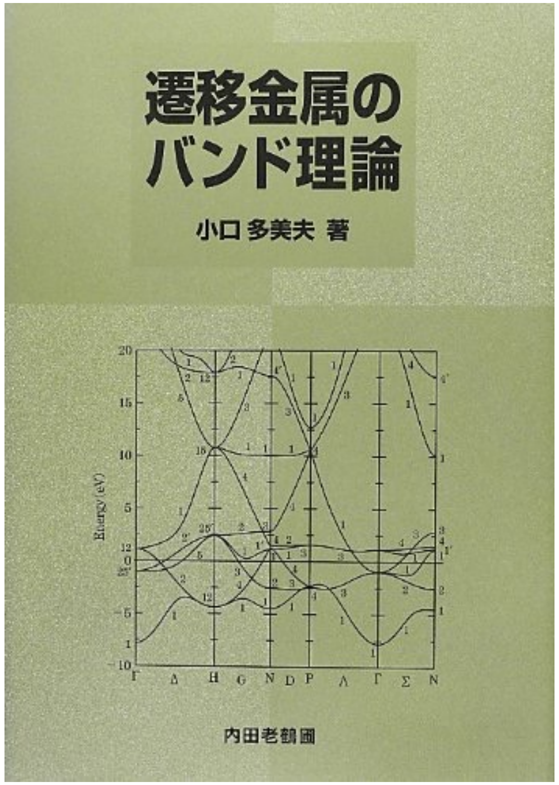
# Textbook of Band Theory

Materials Series
堂山昌男
小川恵一 北田正弘
監修

小口 多美夫 著

バンド理論
物質科学の基礎として

内田老鶴圃



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内田老鶴圃　1999年

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内田老鶴圃　2012年

# Bloch Function

$$T(\mathbf{R})\psi_j^{\mathbf{k}}(\mathbf{r}) = \psi_j^{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_j^{\mathbf{k}}(\mathbf{r})$$ **: Bloch theorem**

$$\psi_j^{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_j^{\mathbf{k}}(\mathbf{r})$$

$$u_j^{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_j^{\mathbf{k}}(\mathbf{r})$$

**: periodic function represented in a Fourier form**

⬇

$$\psi_j^{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{\mathbf{K}} a_{j,\mathbf{K}}^{\mathbf{k}} e^{i\mathbf{K}\cdot\mathbf{r}}$$

$$= \sum_{\mathbf{K}} a_{j,\mathbf{K}}^{\mathbf{k}} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}$$

**K: reciprocal lattice**

# Bloch Function

- **Normalized in a macroscopic volume Ω**
- **k points in BZ are independent and sufficient**

$$\psi_j^{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{K}} a_j^{\mathbf{k}+\mathbf{K}} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}$$

⇓

$$\mathcal{H}\psi_j^{\mathbf{k}}(\mathbf{r}) = \varepsilon_j^{\mathbf{k}} \psi_j^{\mathbf{k}}(\mathbf{r})$$

# Secular Equation

$$\sum_{\mathbf{K}} \langle \mathbf{k}+\mathbf{K}' | \mathcal{H} - \varepsilon_j^{\mathbf{k}} | \mathbf{k}+\mathbf{K} \rangle a_j^{\mathbf{k}+\mathbf{K}} = 0$$

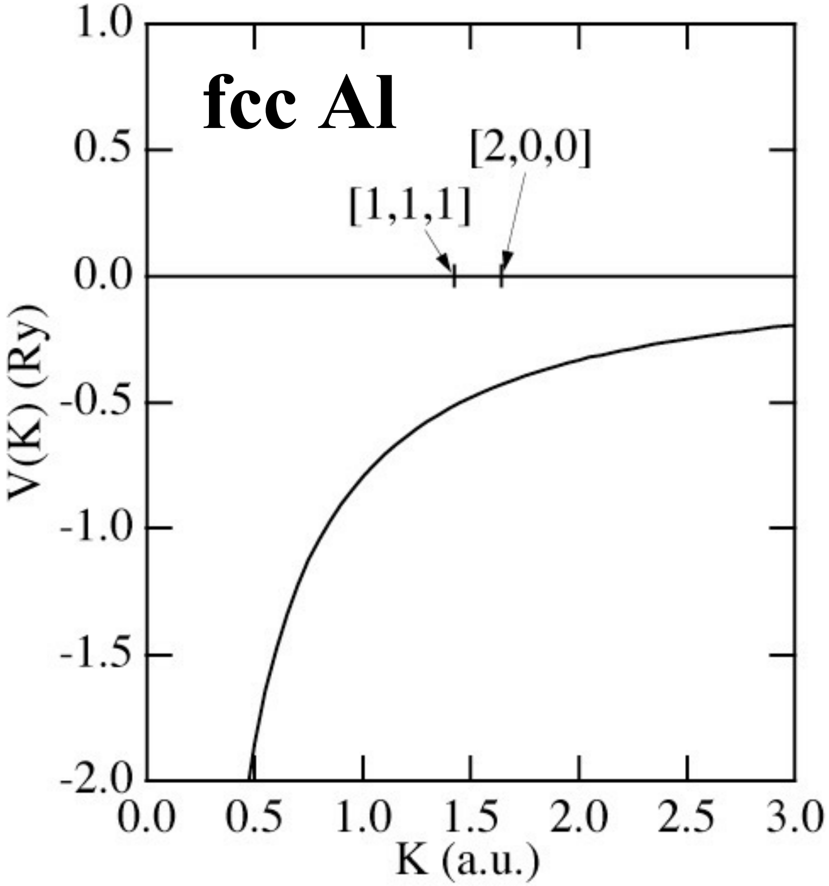
## Matrix elements

$$\langle \mathbf{k}+\mathbf{K}' | \mathcal{H} | \mathbf{k}+\mathbf{K} \rangle = \frac{\hbar^2}{2m} |\mathbf{k}+\mathbf{K}|^2 \delta_{\mathbf{K}',\mathbf{K}} + V(\mathbf{K}'-\mathbf{K})$$

$$V(\mathbf{K}'-\mathbf{K}) = \frac{1}{\Omega} \int d\mathbf{r} e^{-i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{r}} v(\mathbf{r})$$

# Fourier Transform of Potential

$$V(\mathbf{K}' - \mathbf{K}) = \frac{1}{\Omega} \int d\mathbf{r} e^{-i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{r}} v(\mathbf{r})$$



$$v(\mathbf{r}) \approx \sum_{\mathbf{R}} v_{\mathrm{atom}}(|\mathbf{r} - \mathbf{R}|)$$

- Very slow convergency of FT of the Coulomb potential requires a large number of K vectors.
- Asymptotic behavior ~ $K^{-2}$.

# Core Functions

$$\langle \mathbf{k}+\mathbf{K}|\phi_{\mathrm{core}}\rangle = \frac{1}{\Omega}\int d\mathbf{r} e^{-i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}\phi_{\mathrm{core}}(\mathbf{r})$$

**Very slow convergency of the core functions because of localized nature.**

# How to Solve the Problems

- **Contributions from core (nucleus and core electron potentials, and orthogonality to core electron states) are replaced by a soft (easily Fourier transformed) potential**

**→ Pseudopotential**

- **PW basis functions are augmented with more localized functions**

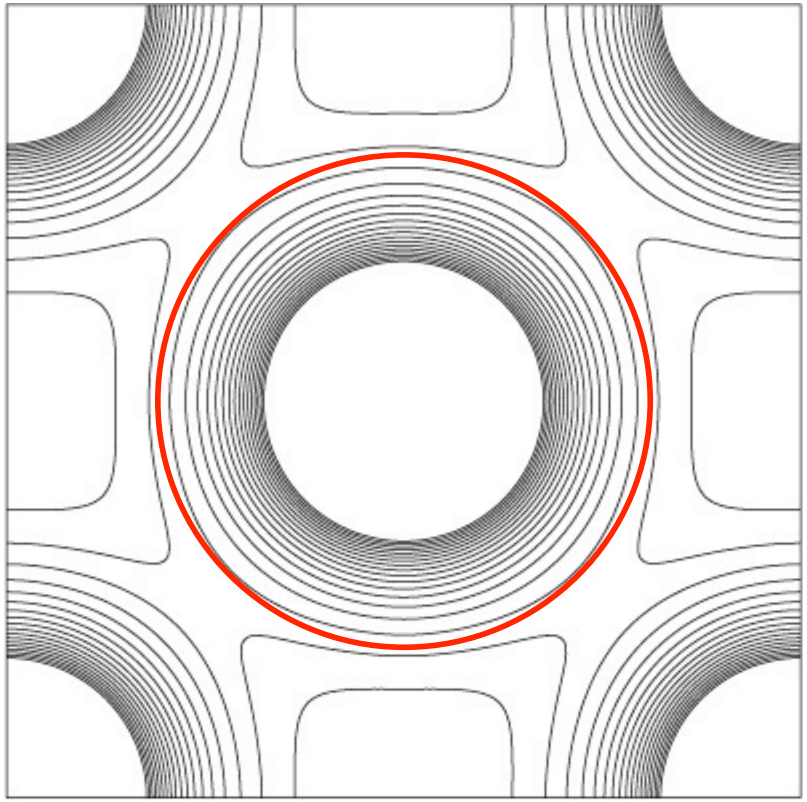
**→ Augmented or mixed basis**

- **Green's functions are used as a multiple scattering problem.**

**→ Koringa-Kohn-Rostoker method**

# Muffin-tin Potential Approximation

- **Spherical around atoms**
- **Constant in the interstitial**



**FCC Cu**

$$v(\mathbf{r}) = \begin{cases} v(|\mathbf{r}-\mathbf{R}|) & |\mathbf{r}-\mathbf{R}| \in S \\ v_{\mathrm{MTZ}} & |\mathbf{r}-\mathbf{R}| \ni S \end{cases}$$

# Slater's Idea

J.C. Slater, PR 51(1937)846.

**Plane waves**

$$|\mathbf{r}-\mathbf{R}| \ni S$$

$$\phi^{\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}$$

**Augmentation waves**

$$|\mathbf{r}-\mathbf{R}| \in S$$

$$\phi^{\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{lm} i^l a_{lm}^{\mathbf{k}+\mathbf{K}} R_l(|\mathbf{r}-\mathbf{R}|;E) Y_{lm}(\mathbf{r}-\mathbf{R})$$

$R_l(r;E)$ **: radial function for energy *E***

$Y_{lm}(\mathbf{r})$ **: spherical harmonics**

# Augmented Plane Wave

J.C. Slater, PR 51(1937)846.

## Secular Equation

$$\det \| \langle \mathbf{k}+\mathbf{K}' | \mathcal{H} - E | \mathbf{k}+\mathbf{K} \rangle \| = 0$$

$$\langle \mathbf{k}+\mathbf{K}' | \mathcal{H} - E | \mathbf{k}+\mathbf{K} \rangle = \left\{ \frac{\hbar^2}{2m} |\mathbf{k}+\mathbf{K}|^2 - E \right\} \delta_{\mathbf{K}',\mathbf{K}}$$

$$+\Gamma^{\mathrm{APW}}_{\mathbf{K}',\mathbf{K}}(E)$$

**Matrix elements have non-linear energy dependence due to logarithmic derivatives of the radial functions.**

**→ Matrix diagonalization scheme cannot be used.**

**→ Need to search the poles of the determinant.**

# Problems in APW Method

1. **Energy dependence of the matrix elements $\Gamma^{\mathrm{APW}}_{\mathbf{K}',\mathbf{K}}(E)$ requires to search poles of the determinant.**

   → **Linear method by Andersen (1975) and**
   **Koelling-Arbman (1975)**

   **L + APW → LAPW**

2. **Muffin-tin potential approximation doesn’t work for less-packing or low-symmetry systems.**

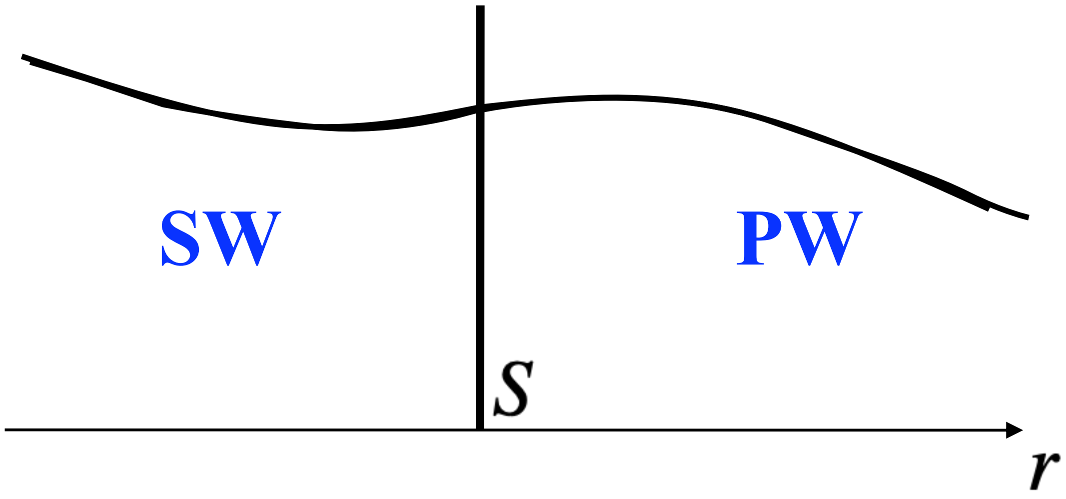
   **Full-potential method by Weinert (1981)**

   → **F + LAPW → FLAPW**

# Logarithmic Derivative

$$L_l(E) = \frac{R_l'(S;E)}{R_l(S;E)} = \frac{d}{dr} \ln R_l(r;E)\Big|_{r=S}$$

**The APW eigenfunction satisfies the boundary conditions (logarithmic derivatives) on the spheres among the general solutions.**



# Single-MT Problem

**Radial Equation in Rydberg units**

$$\left[-\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}+\frac{l(l+1)}{r^2}+v(r)-E\right]R_l(r;E)=0$$

**Normalization** $\int_0^S R_l^2(r;E)r^2dr=1$

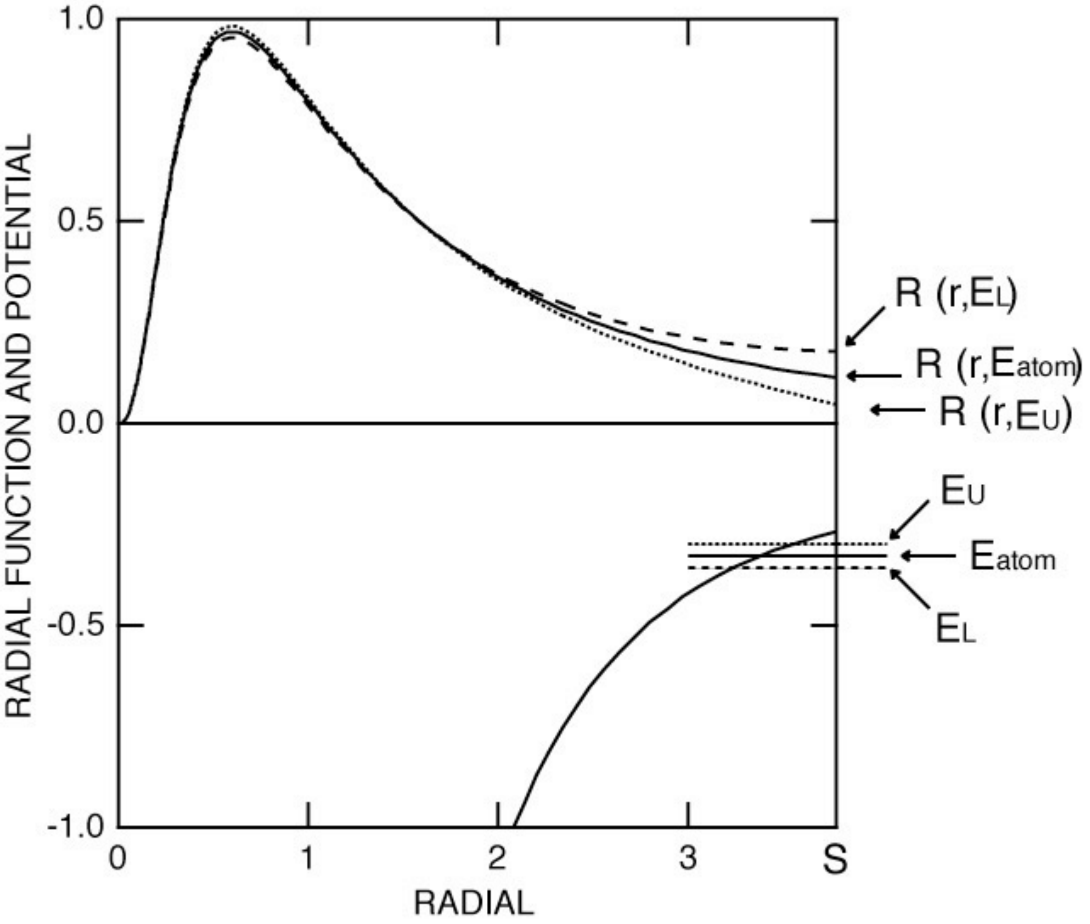
**Radial function** $P_l(r;E)=rR_l(r;E)$

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+v(r)-E\right]P_l(r;E)=0$$

$$\int_0^S P_l^2(r;E)dr=1$$

# Energy Dependence of Radial Function

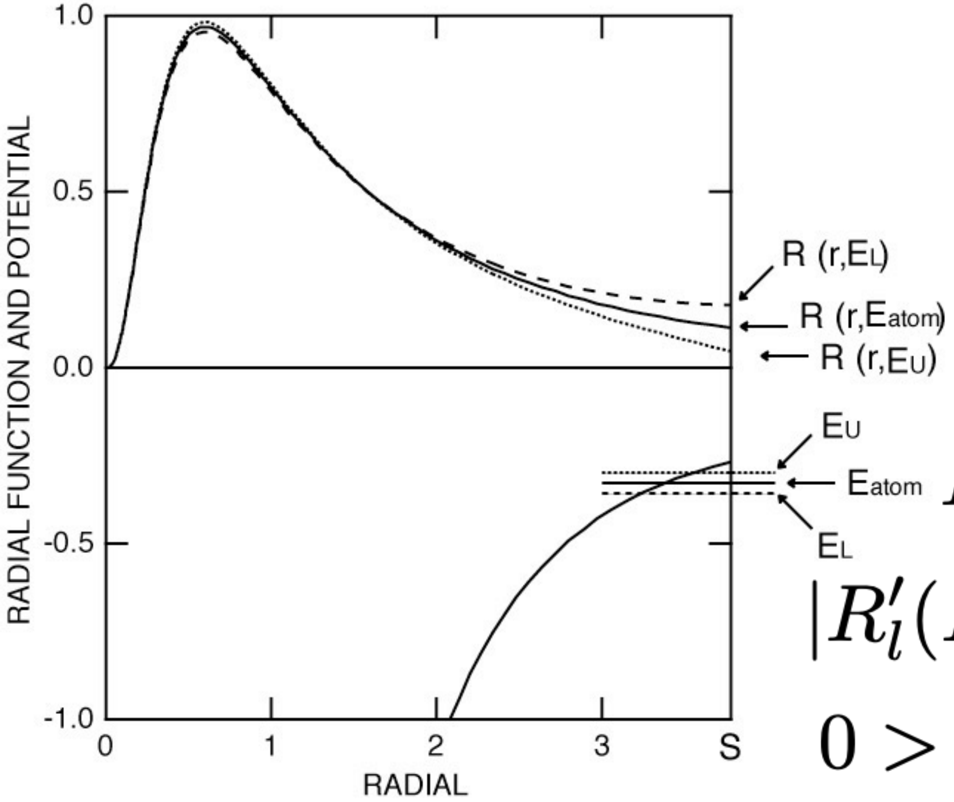
$$\frac{d^2 P_l(r;E)}{dr^2} = \left[\frac{l(l+1)}{r^2} + v(r) - E\right] P_l(r;E)$$



$$E_L < E_{atom} < E_U$$

# Logarithmic Derivative

$$L_l(E) = \frac{R_l'(S;E)}{R_l(S;E)} = \frac{d}{dr}\ln R_l(r;E)\bigg|_{r=S}$$



$$E_L < E_{atom} < E_U$$

$$R_l(E_L) > R_l(E_{atom}) > R_l(E_U)$$

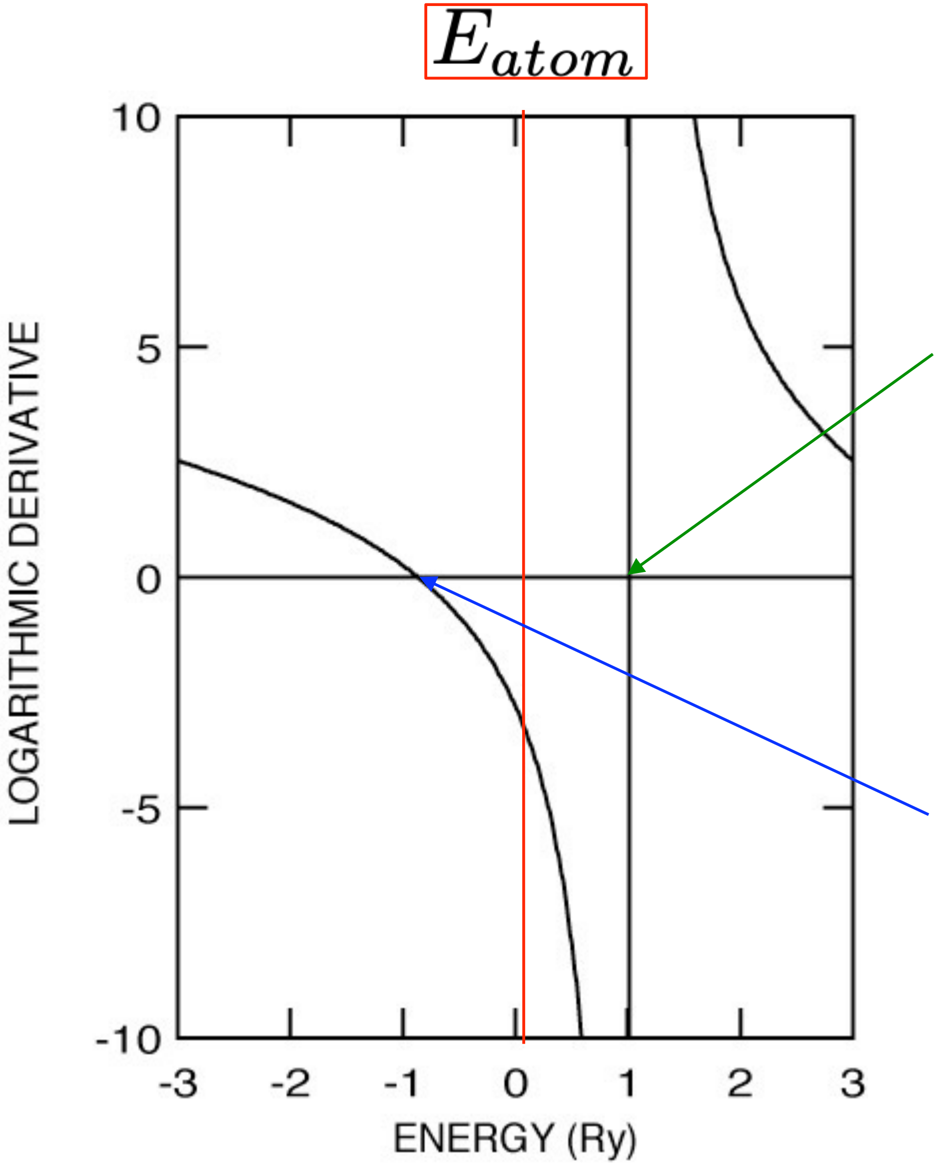
$$|R_l'(E_L)| < |R_l'(E_{atom})| < |R_l'(E_U)|$$

$$0 > L_l(E_L) > L_l(E_{atom}) > L_l(E_U)$$

# Logarithmic Derivative

$L_l(E)$

**bcc W-*d***

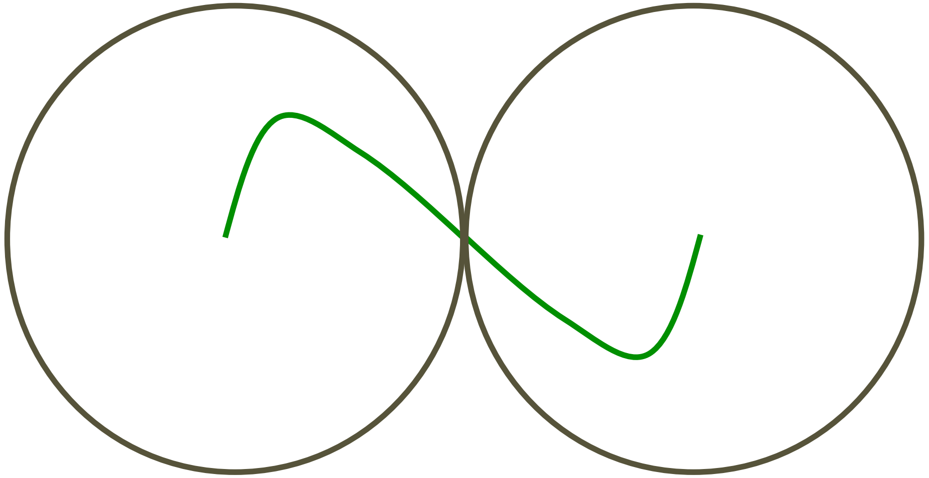


$$\begin{cases} R_l(E_A) = 0 \\ R_l'(E_A) \neq 0 \end{cases}$$

$$\begin{cases} R_l(E_B) \neq 0 \\ R_l'(E_B) = 0 \end{cases}$$

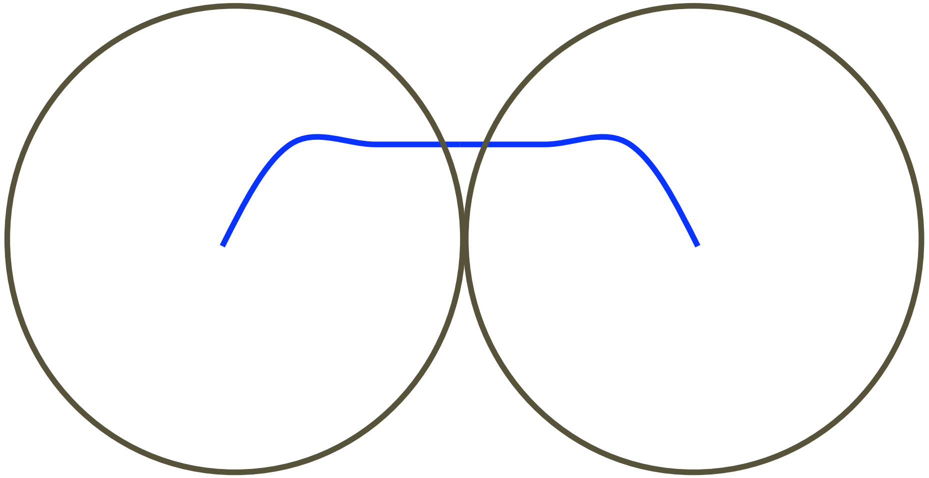
# Logarithmic Derivative

$$\begin{cases} R_l(E_A) = 0 \\ R_l'(E_A) \neq 0 \end{cases}$$



**Anti-bonding state**

$$\begin{cases} R_l(E_B) \neq 0 \\ R_l'(E_B) = 0 \end{cases}$$



**Bonding state**


# Linear Method

**O.K. Andersen, PRB 12(1975)3060.**

**D.D. Koelling and G.O. Arbman, JPF 5(1975)2041.**

- **Remove the energy dependence of radial functions just like a Tayler expansion**

$$R_l(r;E) \approx R_l(r;E_0) + (E-E_0)\dot{R}_l(r;E_0) + \cdots$$

$$\dot{R}_l(r;E_0) = \left. \frac{d}{dE} R_l(r;E) \right|_{E=E_0}$$

- **Use radial function at $E_0$ and its energy derivative to represent a radial function with any logarithmic derivative**

$$R_l(r;D) = R_l(r;E_0) + \omega(D)\dot{R}_l(r;E_0)$$

# Linear Method

- **APW → LAPW**

- **KKR → MTO → LMTO**

  **KKR: Korringa-Kohn-Rostoker**

  **LMTO: Linear Muffin-Tin Orbital**

  **usually combined with ASA***

  ***ASA: Atomic Sphere Approximation**

# LAPW Method

**Augmentation basis**

$$\phi^{\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{lm} i^l \phi_{lm}^{\mathbf{k}+\mathbf{K}}(|\mathbf{r}-\mathbf{R}|) Y_{lm}(\mathbf{r}-\mathbf{R})$$

$$\phi_{lm}^{\mathbf{k}+\mathbf{K}}(r) = A_{lm}^{\mathbf{k}+\mathbf{K}} R_l(r;E_l) + B_{lm}^{\mathbf{k}+\mathbf{K}} \dot{R}_l(r;E_l)$$

$\left\{ \begin{array}{l} A_{lm}^{\mathbf{k}+\mathbf{K}} \\ B_{lm}^{\mathbf{k}+\mathbf{K}} \end{array} \right.$ **determined from the boundary conditions**

$E_l$ **energy parameter usually taken at the center of the occupied partial band**

# LAPW Method

$$A_{lm}^{\mathbf{k}+\mathbf{K}} = 4\pi S^2 a_l^{\mathbf{k}+\mathbf{K}} Y_{lm}^*(\mathbf{k}+\mathbf{K})$$

$$B_{lm}^{\mathbf{k}+\mathbf{K}} = 4\pi S^2 b_l^{\mathbf{k}+\mathbf{K}} Y_{lm}^*(\mathbf{k}+\mathbf{K})$$

$$a_l^{\mathbf{k}+\mathbf{K}} = |\mathbf{k}+\mathbf{K}| j'_{l\mathbf{K}} \dot{R}_l - j_{l\mathbf{K}} \dot{R}'_l$$

$$b_l^{\mathbf{k}+\mathbf{K}} = j_{l\mathbf{K}} R'_l - |\mathbf{k}+\mathbf{K}| j_{l\mathbf{K}} R_l$$

**PW → Spherical Bessel ft.**

$$j_{l\mathbf{K}} = j_l(|\mathbf{k}+\mathbf{K}|S) \qquad j'_{l\mathbf{K}} = \left.\frac{dj_l(x)}{dx}\right|_{x=|\mathbf{k}+\mathbf{K}|S}$$

$$R_l = R_l(S; E_l)$$

# Matrix Elements in LAPW

in Rydberg atomic units

$$\mathbf{H}\mathbf{C} = \mathbf{S}\mathbf{C}E$$

$$\begin{aligned}
H_{\mathbf{K}',\mathbf{K}} &= \langle \mathbf{k}+\mathbf{K}' | \mathcal{H} | \mathbf{k}+\mathbf{K} \rangle \\
&= (\mathbf{k}+\mathbf{K}')\cdot(\mathbf{k}+\mathbf{K})U(\mathbf{K}'-\mathbf{K}) \\
&\quad + \frac{4\pi S^4}{\Omega_0}\sum_l (2l+1)P_l\left((\mathbf{k}+\mathbf{K}')\cdot(\mathbf{k}+\mathbf{K})\right) \\
&\qquad \times \left(E_l s_l^{\mathbf{K}',\mathbf{K}} + \gamma_l^{\mathbf{K}',\mathbf{K}}\right)
\end{aligned}$$

$$\begin{aligned}
S_{\mathbf{K}',\mathbf{K}} &= \langle \mathbf{k}+\mathbf{K}' | \mathbf{k}+\mathbf{K} \rangle \\
&= U(\mathbf{K}'-\mathbf{K}) \\
&\quad + \frac{4\pi S^4}{\Omega_0}\sum_l (2l+1)P_l\left((\mathbf{k}+\mathbf{K}')\cdot(\mathbf{k}+\mathbf{K})\right) s_l^{\mathbf{K}',\mathbf{K}}
\end{aligned}$$

# Matrix Elements in LAPW

in Rydberg atomic units

$$U(\mathbf{K}) = \delta_{\mathbf{K}} - \frac{4\pi S^2}{\Omega_0}\frac{j_1(KS)}{K}$$

$$s_l^{\mathbf{K}',\mathbf{K}} = a_l^{\mathbf{k}+\mathbf{K}'}a_l^{\mathbf{k}+\mathbf{K}} + b_l^{\mathbf{k}+\mathbf{K}'}b_l^{\mathbf{k}+\mathbf{K}}N_l$$

$$N_l = \int_0^S \dot{R}_l^2(r;E_l)r^2dr$$

$$\gamma_l^{\mathbf{K}',\mathbf{K}} = \dot{R}_l R_l' \left\{|\mathbf{k}+\mathbf{K}|j_{l\mathbf{K}}'j_{l\mathbf{K}'} + |\mathbf{k}+\mathbf{K}'|j_{l\mathbf{K}}j_{l\mathbf{K}'}'\right\}$$

$$-\left\{\dot{R}_l'R_l'j_{l\mathbf{K}}j_{l\mathbf{K}'} + \dot{R}_l R_l|\mathbf{k}+\mathbf{K}||\mathbf{k}+\mathbf{K}'|j_{l\mathbf{K}}'j_{l\mathbf{K}'}'\right\}$$

# Why the Linear Method Works Well?

## Orthogonality to maximize the variational degree

$$\int_0^S R_l(r;E_l)\dot{R}_l(r;E_l)r^2dr = 0$$

## Orthogonality to the core functions

$$\int_0^S R_l(r;E_l)R_{\text{core}}(r;E_{\text{core}})r^2dr = 0$$

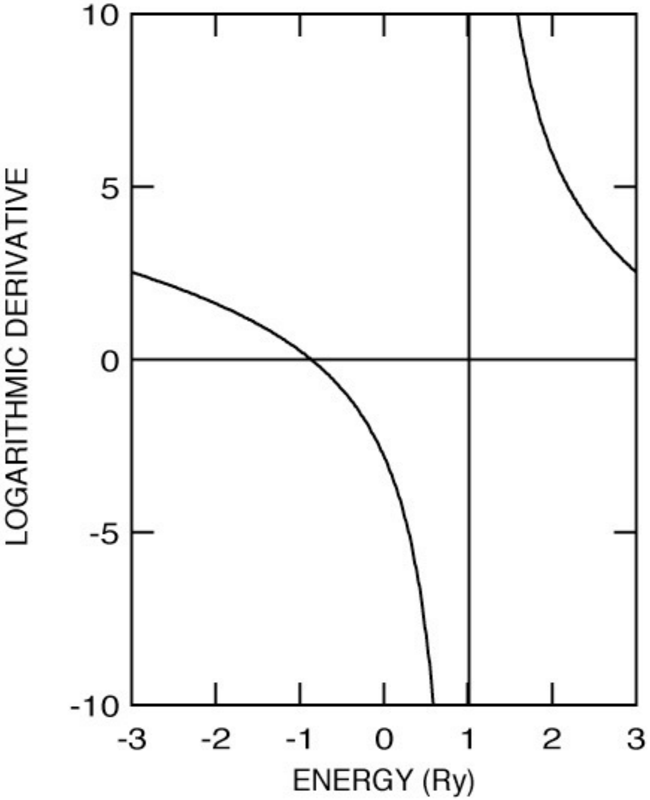
$$\int_0^S \dot{R}_l(r;E_l)R_{\text{core}}(r;E_{\text{core}})r^2dr = 0$$

# Why the Linear Method Works Well?

**Energy expectation value of the orbital with the exact logarithmic derivative**

$$\langle E(D)\rangle = \frac{\langle \phi_l(D)|\mathcal{H}|\phi_l(D)\rangle_S}{\langle \phi_l(D)|\phi_l(D)\rangle_S}$$

$$= E + \mathcal{O}(E - E_l)^4$$



# Coulomb Potential

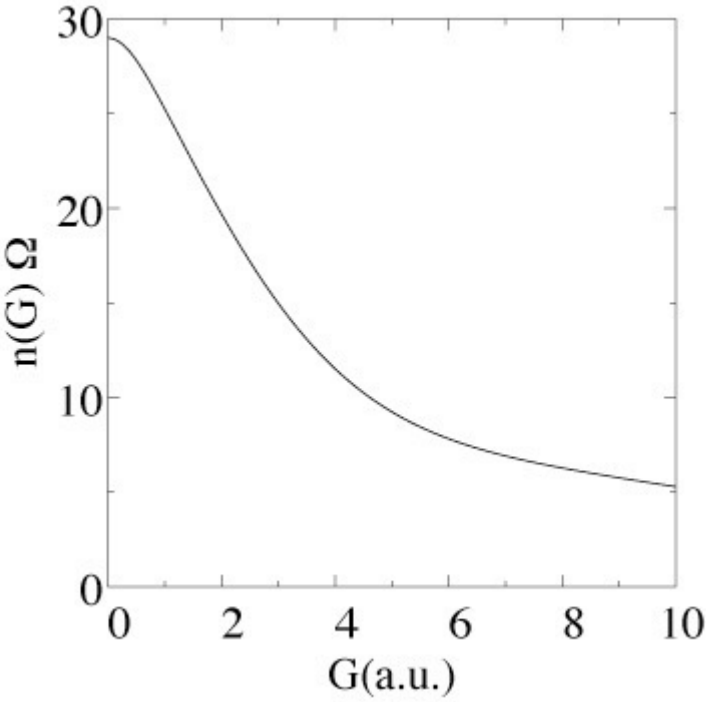
- **Coulomb potential for smooth density distribution**

$$n(\mathbf{r}) = \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} n_{\mathbf{G}} \qquad \nabla^2 v^{\mathrm{C}}(\mathbf{r}) = 4\pi e^2 n(\mathbf{r})$$

$$v^{\mathrm{C}}(\mathbf{r}) = \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} v^{\mathrm{C}}_{\mathbf{G}} \qquad v^{\mathrm{C}}_{\mathbf{G}} = \frac{4\pi e^2 n_{\mathbf{G}}}{G^2}$$

- **Realistic distribution**

$$n_{\mathbf{G}} = \frac{1}{\Omega} \int e^{-i\mathbf{G}\cdot\mathbf{r}} n(\mathbf{r}) d\mathbf{r}$$



# Full-potential Method

**M. Weinert, J. Math. Phys. 22 (1981) 2433.**

- **Electron density inside the sphere is replaced by a smoothed density with the exact multipole moments.**

$$n(\mathbf{r}) = \begin{cases} \tilde{n}(\mathbf{r}) & |\mathbf{r}-\mathbf{R}| \in S \\ n(\mathbf{r}) & |\mathbf{r}-\mathbf{R}| \ni S \end{cases}$$

- **Potential outside the sphere is given with the smoothed density.**
- **Potential inside the sphere can be solved with the sphere boundary conditions.**

# Full-potential Method

- **Pseudized density inside the sphere**

$$\tilde{n}(\mathbf{r}) = \sum_{lm} Q_{lm} Y_{lm} \sum_{\eta} a_{\eta} r^{\nu_{\eta}}$$

$$\tilde{n}_{\mathbf{G}} = \frac{4\pi}{\Omega_0} \sum_{lm} \frac{(-i)^l (2l+2n+3)!!}{(2l+1)!! S^l}$$

$$\times \frac{j_{l+n+1}(GS)}{(GS)^{n+1}} \boxed{q_{lm}} Y_{lm}(\mathbf{G})$$

**multipole moments**

# Full-potential Method

- **Potential inside the sphere**

**potential on sphere**

$$v^{\mathrm{C}}(\mathbf{r}) = \int_S n(\mathbf{r}')G(\mathbf{r},\mathbf{r}')d\mathbf{r}' - \frac{S^2}{4\pi}\oint_S \boxed{v^{\mathrm{C}}(\mathbf{S})}\nabla G \cdot d\mathbf{S}$$

$$G(\mathbf{r},\mathbf{r}') = 4\pi \sum_{lm} \frac{Y^*_{lm}(\mathbf{r}')Y_{lm}(\mathbf{r})}{2l+1}\frac{r^l_<}{r^{l+1}_>}\left[1-\left(\frac{r_>}{S}\right)^{2l+1}\right]$$

$$\nabla G \cdot \hat{n} = -\frac{4\pi}{S^2}\sum_{lm}\left(\frac{r}{S}\right)^l Y^*_{lm}(\mathbf{r}')Y_{lm}(\mathbf{r})$$

# Full-potential Method

- **Electron density inside the sphere**

$$n(\mathbf{r}) = \sum_{lm} n_{lm}(r) Y_{lm}(\mathbf{r})$$

- **Potential function inside the sphere**

$$v(\mathbf{r}) = \sum_{lm} v_{lm}(r) Y_{lm}(\mathbf{r})$$

- **Matrix element of potential**

$$\Delta H_{\mathbf{K}',\mathbf{K}} = \langle \mathbf{k} + \mathbf{K}' | \boxed{\Delta v} | \mathbf{k} + \mathbf{K} \rangle$$

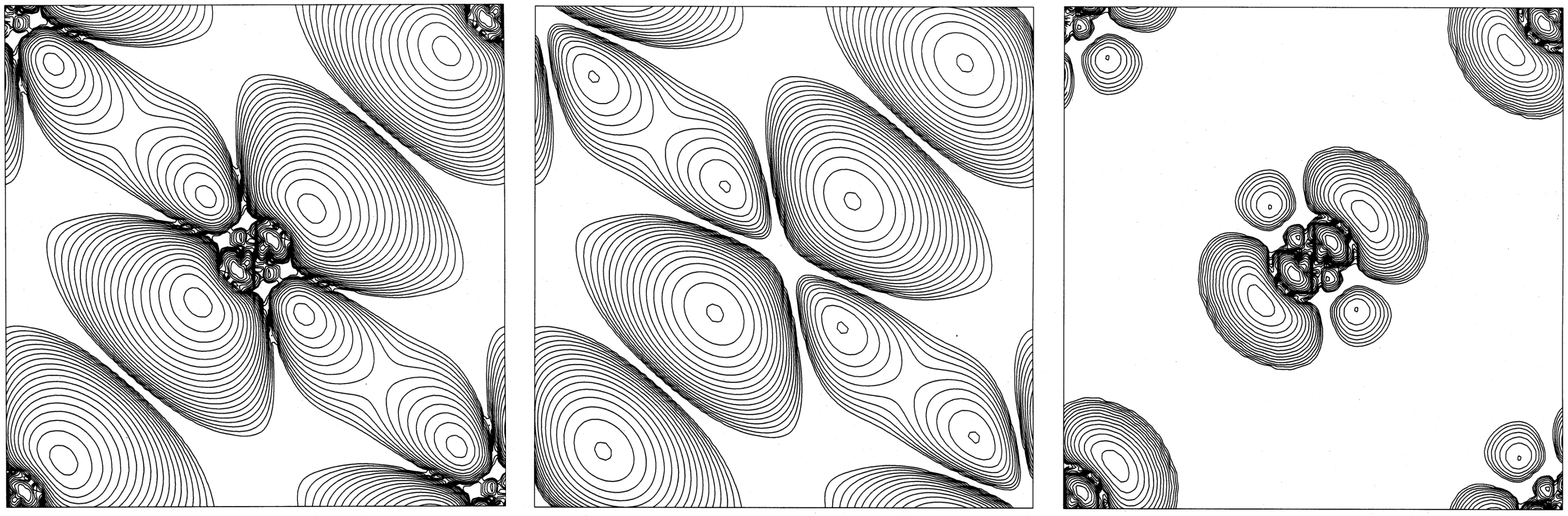
**non-spherical part**

# FLAPW Method

- Two-dimensional slab models
  - E. Wimmer, H. Krakauer, M. Weinert and A.J. Freeman, PRB 24 (1981) 864.
  - M. Weinert, E. Wimmer and A.J. Freeman, PRB 26 (1982) 4571.
- Three-dimensional systems
  - H.J.F. Jansen and A.J. Freeman, PRB 30 (1984) 561.

# FLAPW Packages Open to Public

$$\psi_j^{\mathbf{k}} = \tilde{\psi}_j^{\mathbf{k}} + \sum_{\nu} \left[ \psi_{\nu j}^{\mathbf{k}} - \tilde{\psi}_{\nu j}^{\mathbf{k}} \right]$$



- **ABCAP**
- **HiLAPW**
- **KANSAI**
- **FLEUR**
- **QMD-FLAPW**
- **WIEN**

# SUMMARY

## FLAPW Method

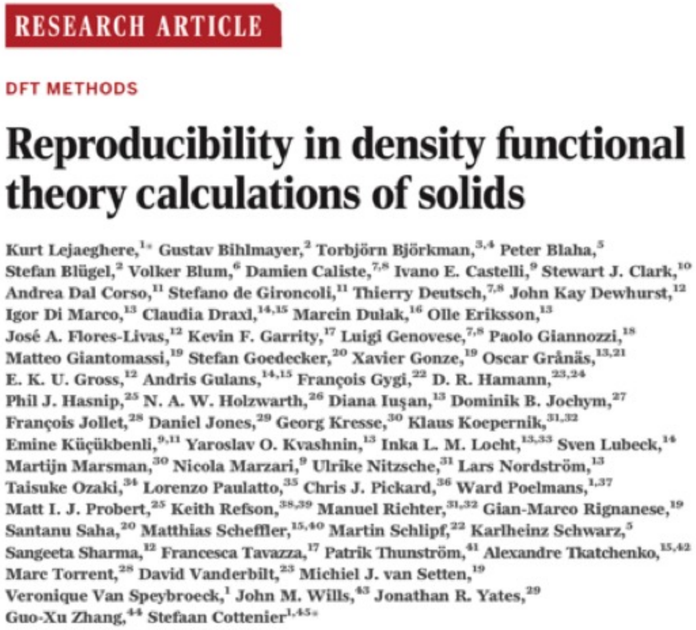
- APW method by Slater
- Linear method by Andersen and Koelling-Arbman
- Full-potential method by Weinert

Highly-Precise All-electron Method

↓

General-purpose first-principles method
for a variety of condensed matter systems

# All-Electron vs. Pseudopotential



RESEARCH ARTICLE

DFT METHODS

## Reproducibility in density functional theory calculations of solids

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Taisuke Ozaki,[34] Lorenzo Paulatto,[35] Chris J. Pickard,[36] Ward Poelmans,[1,37]
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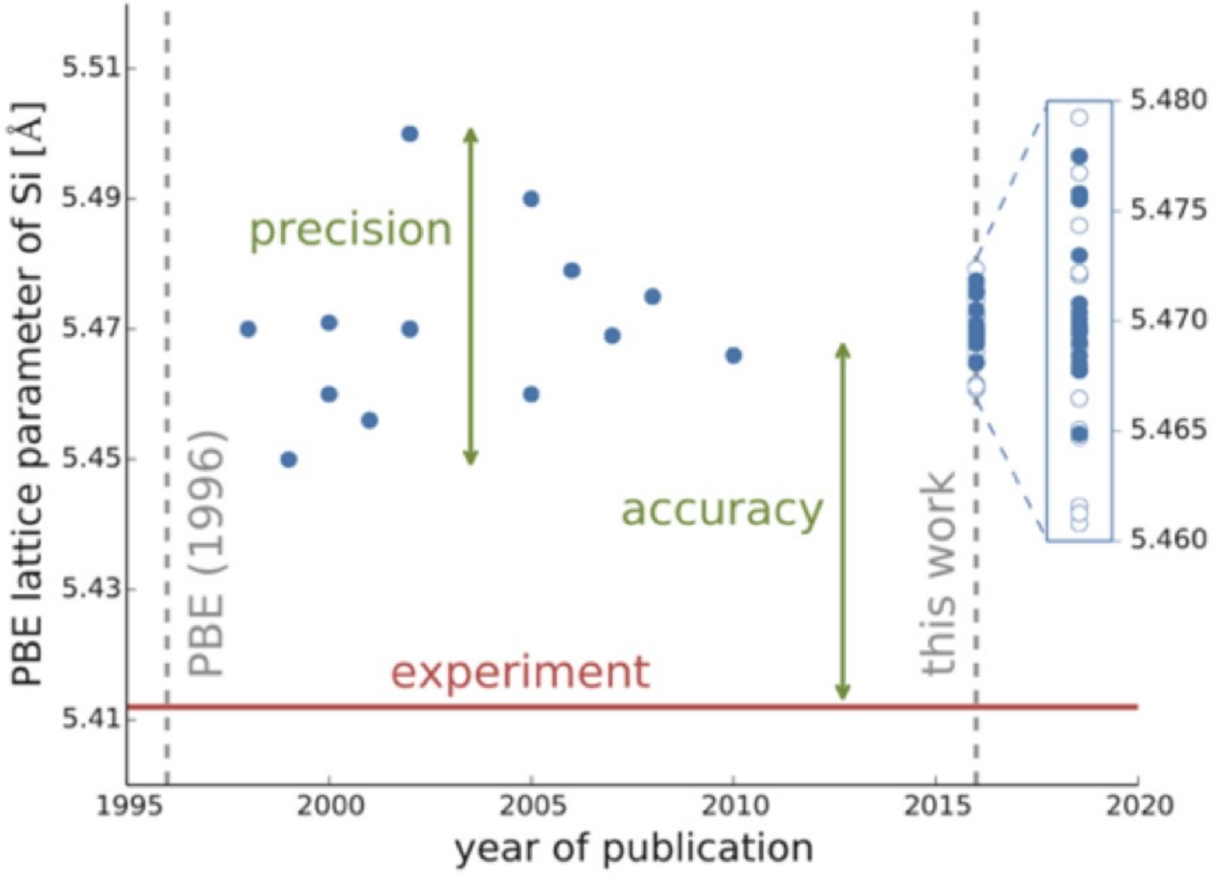
Santanu Saha,[20] Matthias Scheffler,[15,40] Martin Schlipf,[22] Karlheinz Schwarz,[5]
Sangeeta Sharma,[12] Francesca Tavazza,[17] Patrik Thunström,[41] Alexandre Tkatchenko,[15,42]
Marc Torrent,[28] David Vanderbilt,[23] Michiel J. van Setten,[19]
Veronique Van Speybroeck,[1] John M. Wills,[43] Jonathan R. Yates,[29]
Guo-Xu Zhang,[44] Stefaan Cottenier[1,45*]



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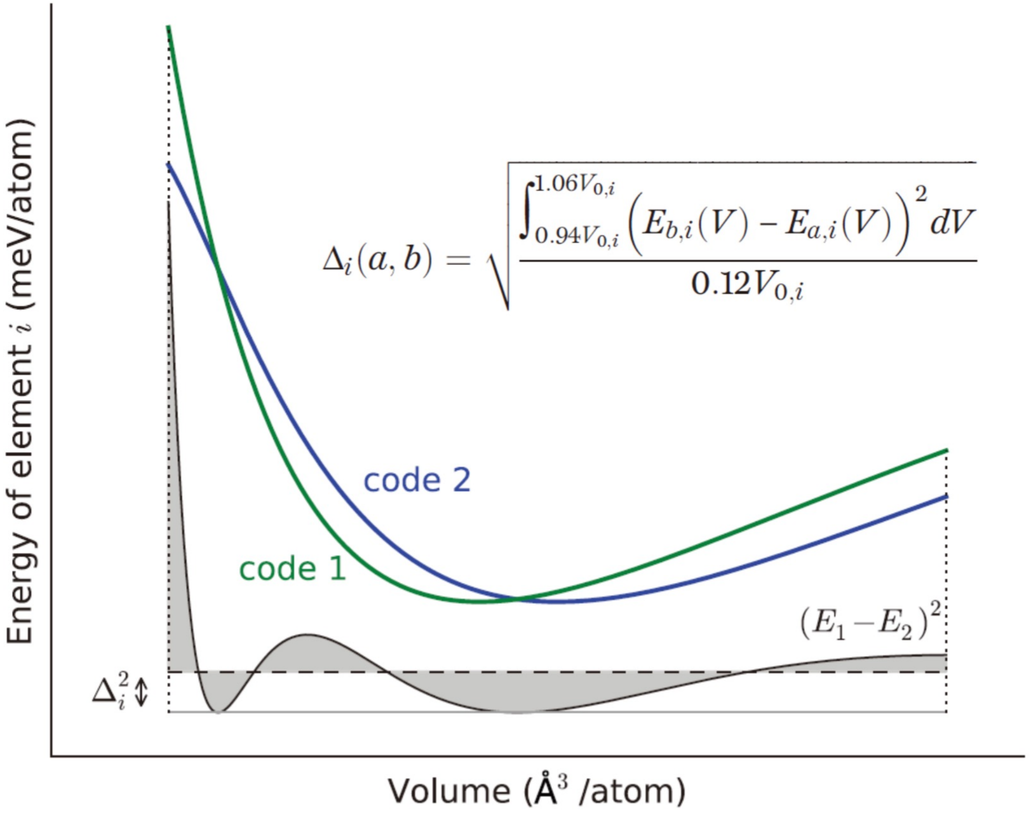
# All-Electron vs. Pseudopotential

## Δ-gauge



$$\Delta_i(a,b)=\sqrt{\frac{\int_{0.94V_{0,i}}^{1.06V_{0,i}}\left(E_{b,i}(V)-E_{a,i}(V)\right)^2 dV}{0.12V_{0,i}}}$$

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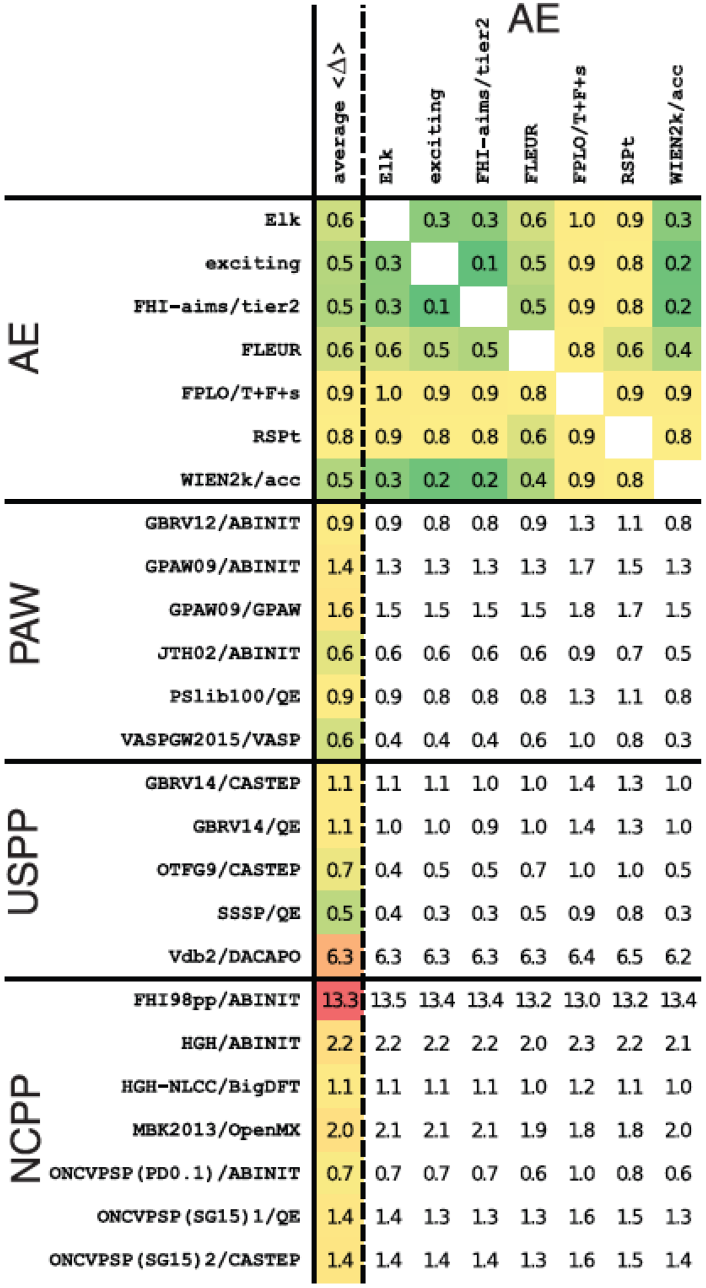
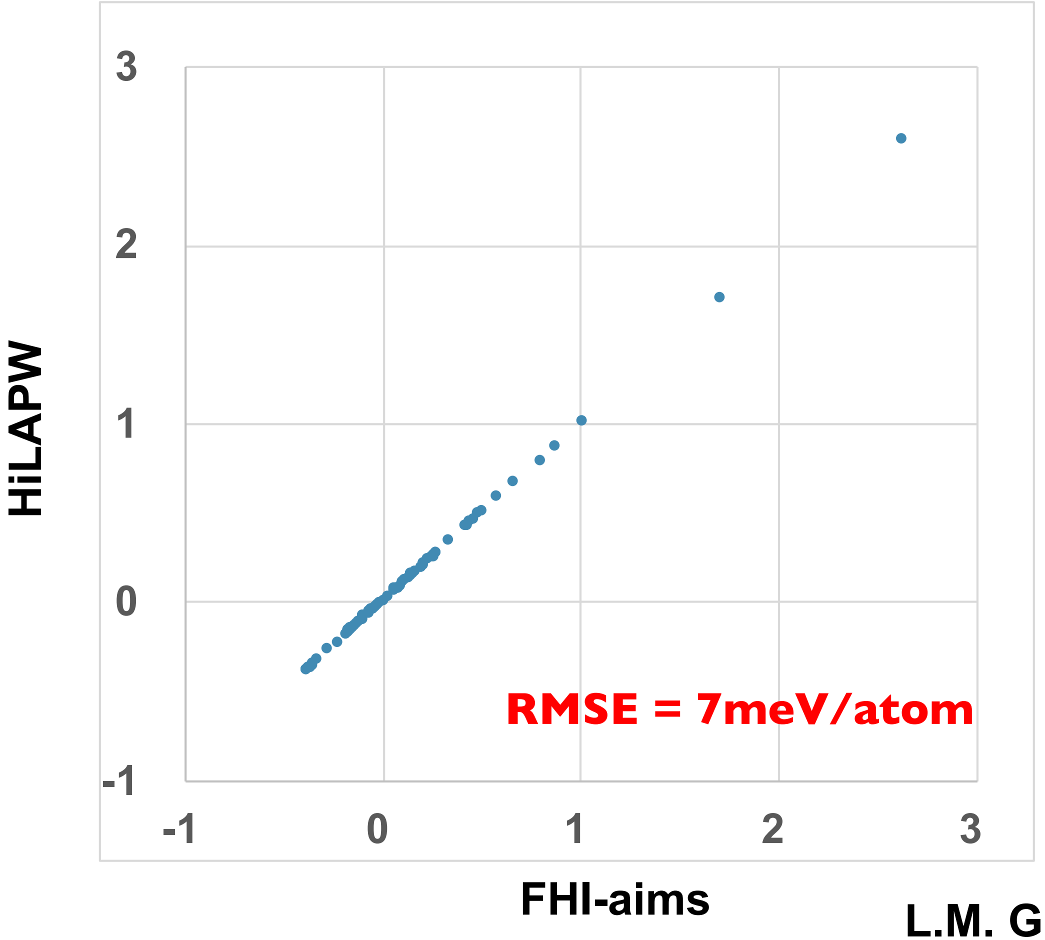


| | | | AE | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | average <Δ> | Elk | exciting | FHI-aims/tier2 | FLEUR | FPLO/T+F+s | RSPt | WIEN2k/acc |
| AE | Elk | 0.6 | | 0.3 | 0.3 | 0.6 | 1.0 | 0.9 | 0.3 |
| | exciting | 0.5 | 0.3 | | 0.1 | 0.5 | 0.9 | 0.8 | 0.2 |
| | FHI-aims/tier2 | 0.5 | 0.3 | 0.1 | | 0.5 | 0.9 | 0.8 | 0.2 |
| | FLEUR | 0.6 | 0.6 | 0.5 | 0.5 | | 0.8 | 0.6 | 0.4 |
| | FPLO/T+F+s | 0.9 | 1.0 | 0.9 | 0.9 | 0.8 | | 0.9 | 0.9 |
| | RSPt | 0.8 | 0.9 | 0.8 | 0.8 | 0.6 | 0.9 | | 0.8 |
| | WIEN2k/acc | 0.5 | 0.3 | 0.2 | 0.2 | 0.4 | 0.9 | 0.8 | |
| PAW | GBRV12/ABINIT | 0.9 | 0.9 | 0.8 | 0.8 | 0.9 | 1.3 | 1.1 | 0.8 |
| | GPAW09/ABINIT | 1.4 | 1.3 | 1.3 | 1.3 | 1.3 | 1.7 | 1.5 | 1.3 |
| | GPAW09/GPAW | 1.6 | 1.5 | 1.5 | 1.5 | 1.5 | 1.8 | 1.7 | 1.5 |
| | JTH02/ABINIT | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | 0.9 | 0.7 | 0.5 |
| | PSlib100/QE | 0.9 | 0.9 | 0.8 | 0.8 | 0.8 | 1.3 | 1.1 | 0.8 |
| | VASPGW2015/VASP | 0.6 | 0.4 | 0.4 | 0.4 | 0.6 | 1.0 | 0.8 | 0.3 |
| USPP | GBRV14/CASTEP | 1.1 | 1.1 | 1.1 | 1.0 | 1.0 | 1.4 | 1.3 | 1.0 |
| | GBRV14/QE | 1.1 | 1.0 | 1.0 | 0.9 | 1.0 | 1.4 | 1.3 | 1.0 |
| | OTFG9/CASTEP | 0.7 | 0.4 | 0.5 | 0.5 | 0.7 | 1.0 | 1.0 | 0.5 |
| | SSSP/QE | 0.5 | 0.4 | 0.3 | 0.3 | 0.5 | 0.9 | 0.8 | 0.3 |
| | Vdb2/DACAPO | 6.3 | 6.3 | 6.3 | 6.3 | 6.3 | 6.4 | 6.5 | 6.2 |
| NCPP | FHI98pp/ABINIT | 13.3 | 13.5 | 13.4 | 13.4 | 13.2 | 13.0 | 13.2 | 13.4 |
| | HGH/ABINIT | 2.2 | 2.2 | 2.2 | 2.2 | 2.0 | 2.3 | 2.2 | 2.1 |
| | HGH-NLCC/BigDFT | 1.1 | 1.1 | 1.1 | 1.1 | 1.0 | 1.2 | 1.1 | 1.0 |
| | MBK2013/OpenMX | 2.0 | 2.1 | 2.1 | 2.1 | 1.9 | 1.8 | 1.8 | 2.0 |
| | ONCVPSP(PD0.1)/ABINIT | 0.7 | 0.7 | 0.7 | 0.7 | 0.6 | 1.0 | 0.8 | 0.6 |
| | ONCVPSP(SG15)1/QE | 1.4 | 1.4 | 1.3 | 1.3 | 1.3 | 1.6 | 1.5 | 1.3 |
| | ONCVPSP(SG15)2/CASTEP | 1.4 | 1.4 | 1.4 | 1.4 | 1.3 | 1.6 | 1.5 | 1.4 |

# FLAPW — Precision

## 82 Octet elementary and binary systems with typical elements

$$\Delta E = E(\mathrm{RS}) - E(\mathrm{ZB}) \quad (\mathrm{eV/atom})$$



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**PRL 114, 105503 (2015)**