

Localized basis methods in OpenMX

- Introduction of OpenMX
- Implementation of OpenMX
 - Total energy
 - Pseudopotentials
 - Basis functions
- Δ -gauge

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Nov. 23rd, OpenMX hands-on workshop in KAIST

OpenMX **Open** source package for **M**aterial **eX**plorer

- 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 Mulliken, 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 functions

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.

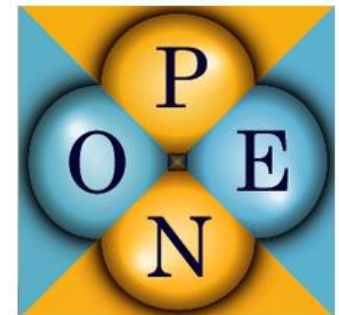
History of OpenMX

- 2000 Start of development
- 2003 Public release (GNU-GPL)
- 2003 Collaboration:
AIST, NIMS, SNU
KAIST, JAIST,
Kanazawa Univ.
CAS, UAM
NISSAN, Fujitsu Labs.
etc.
- 2015 18 public releases
Latest version: 3.8

Welcome to OpenMX
open source package for Material explorer

Contents

- [What's new](#)
 - OpenMX Hands-On Workshop on 10th Oct. in Kobe
 - Patch (Ver.3.7.8) to OpenMX Ver. 3.7 (17/Feb/2014)
 - Release of OpenFFT Ver. 1.0 (04/Sep/2013)
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<http://www.openmx-square.org>

About 400 papers published using OpenMX

Developers of OpenMX

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- M. J. Han (KAIST)
- M. Ohfuti (Fujitsu)
- T. Ohwaki (Nissan)
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- Y.P. Mizuta (Kanazawa Univ.)
- M. Kawamura (Univ. of Tokyo)
- K. Yoshimi (Univ. of Tokyo)

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 $J_{\text{eff}}=1/2$ 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., Phys. 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 400 published papers

Implementation of OpenMX

- Density functional theory
- Mathematical structure of KS eq.
- LCPAO method
- Total energy
- Pseudopotentials
- Basis functions

Density functional theory

The energy of non-degenerate ground state can be expressed by a functional of electron density. (Hohenberg and Kohn, 1964)

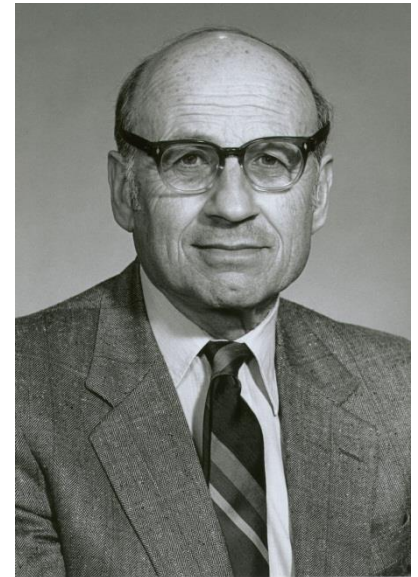
$$E[\rho] = \int \rho(\mathbf{r})v(\mathbf{r})d + T[\rho] + J[\rho] + E_{xc}[\rho]$$

The many body problem of the ground state can be reduced to an one-particle problem with an effective potential. (Kohn-Sham, 1965)

$$\hat{H}_{KS}\phi_i = \varepsilon_i\phi_i$$

$$\hat{H}_{KS} = -\frac{1}{2}\nabla^2 + v_{\text{eff}}$$

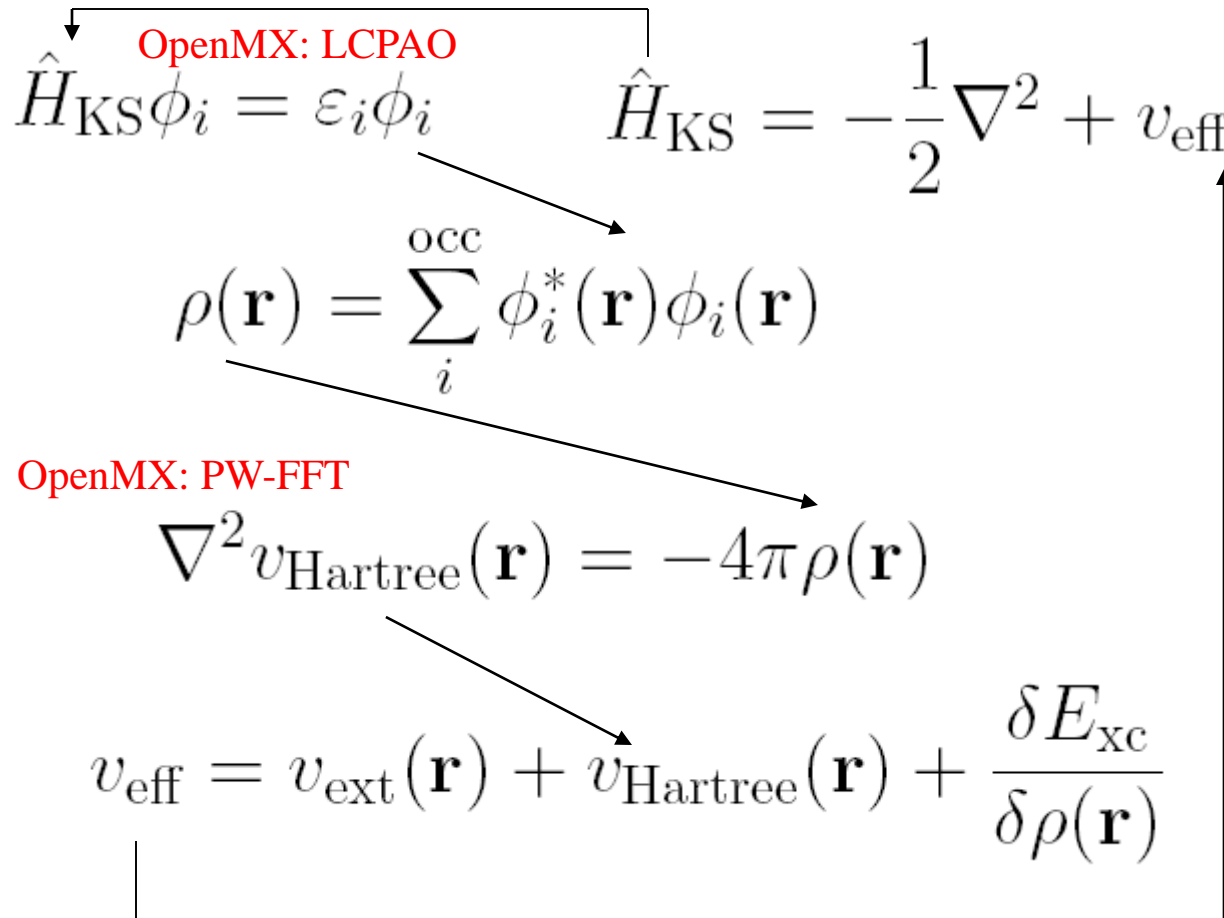
$$v_{\text{eff}} = v_{\text{ext}}(\mathbf{r}) + v_{\text{Hartree}}(\mathbf{r}) + \frac{\delta E_{xc}}{\delta \rho(\mathbf{r})}$$



W.Kohn (1923-)

Mathematical structure of KS eq.

3D coupled non-linear differential equations have to be solved self-consistently.



Input charge = Output charge \rightarrow Self-consistent condition

LCPAO method

(Linear-Combination of Pseudo Atomic Orbital Method)

One-particle KS orbital

$$\psi_{\sigma\mu}^{(\mathbf{k})}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{n}} e^{i\mathbf{R}_{\mathbf{n}} \cdot \mathbf{k}} \sum_{i\alpha} c_{\sigma\mu,i\alpha}^{(\mathbf{k})} \phi_{i\alpha}(\mathbf{r} - \tau_i - \mathbf{R}_{\mathbf{n}}),$$

is expressed by a linear combination of atomic like orbitals in the method.

$$\phi(\mathbf{r}) = Y_l^m(\hat{\mathbf{r}}) R(r)$$

Features:

- It is easy to interpret physical and chemical meanings, since the KS orbitals are expressed by the atomic like basis functions.
- It gives rapid convergent results with respect to basis functions due to physical origin. (however, it is not a complete basis set, leading to difficulty in getting full convergence.)
- The memory and computational effort for calculation of matrix elements are $O(N)$.
- It well matches the idea of linear scaling methods.

➤ Total energy

➤ Pseudopotentials

➤ Basis functions

Implementation: Total energy (1)

The total energy is given by the sum of six terms, and a proper integration scheme for each term is applied to accurately evaluate the total energy.

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{ec}} + E_{\text{ee}} + E_{\text{xc}} + E_{\text{cc}} = E_{\text{kin}} + E_{\text{na}} + E_{\text{ec}}^{(\text{NL})} + E_{\delta\text{ee}} + E_{\text{xc}} + E_{\text{scc}}.$$

$$E_{\text{kin}} = \sum_{\sigma} \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} \rho_{\sigma, i\alpha j\beta}^{(\mathbf{R}_{\mathbf{n}})} h_{i\alpha j\beta, \text{kin}}^{(\mathbf{R}_{\mathbf{n}})}. \quad \text{Kinetic energy}$$

$$\begin{aligned} E_{\text{ec}} &= E_{\text{ec}}^{(\text{L})} + E_{\text{ec}}^{(\text{NL})}, \quad \text{Coulomb energy with external potential} \\ &= \sum_{\sigma} \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} \rho_{\sigma, i\alpha j\beta}^{(\mathbf{R}_{\mathbf{n}})} \langle \phi_{i\alpha}(\mathbf{r} - \tau_i) | \sum_I V_{\text{core}, I}(\mathbf{r} - \tau_I) | \phi_{j\beta}(\mathbf{r} - \tau_j - \mathbf{R}_{\mathbf{n}}) \rangle \\ &\quad + \sum_{\sigma} \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} \rho_{\sigma, i\alpha j\beta}^{(\mathbf{R}_{\mathbf{n}})} \langle \phi_{i\alpha}(\mathbf{r} - \tau_i) | \sum_I V_{\text{NL}, I}(\mathbf{r} - \tau_I) | \phi_{j\beta}(\mathbf{r} - \tau_j - \mathbf{R}_{\mathbf{n}}) \rangle, \end{aligned}$$

$$\begin{aligned} E_{\text{ee}} &= \frac{1}{2} \int d\mathbf{r}^3 n(\mathbf{r}) V_{\text{H}}(\mathbf{r}), \quad \text{Hartree energy} \\ &= \frac{1}{2} \int d\mathbf{r}^3 n(\mathbf{r}) \{ V_{\text{H}}^{(\text{a})}(\mathbf{r}) + \delta V_{\text{H}}(\mathbf{r}) \}, \end{aligned}$$

$$E_{\text{xc}} = \int d\mathbf{r}^3 \{ n_{\uparrow}(\mathbf{r}) + n_{\downarrow}(\mathbf{r}) + n_{\text{pcc}}(\mathbf{r}) \} \epsilon_{\text{xc}}(n_{\uparrow} + \frac{1}{2}n_{\text{pcc}}, n_{\downarrow} + \frac{1}{2}n_{\text{pcc}}), \quad \text{Exchange-correlation energy}$$

$$E_{\text{cc}} = \frac{1}{2} \sum_{I, J} \frac{Z_I Z_J}{|\tau_I - \tau_J|}. \quad \text{Core-core Coulomb energy}$$

Implementation: Total energy (2)

The reorganization of Coulomb energies gives three new energy terms.

$$E_{\text{ec}}^{(L)} + E_{\text{ee}} + E_{\text{cc}} = E_{\text{na}} + E_{\delta\text{ee}} + E_{\text{scc}},$$

The neutral atom energy

$$E_{\text{na}} = \int d\mathbf{r}^3 n(\mathbf{r}) \sum_I V_{\text{na},I}(\mathbf{r} - \tau_I),$$

Short range and separable to two-center integrals

$$= \sum_{\sigma} \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} \rho_{\sigma, i\alpha j\beta}^{(\mathbf{R}_{\mathbf{n}})} \sum_I \langle \phi_{i\alpha}(\mathbf{r} - \tau_i) | V_{\text{na},I}(\mathbf{r} - \tau_I) | \phi_{j\beta}(\mathbf{r} - \tau_j - \mathbf{R}_{\mathbf{n}}) \rangle,$$

Difference charge Hartree energy

$$E_{\delta\text{ee}} = \frac{1}{2} \int d\mathbf{r}^3 \delta n(\mathbf{r}) \delta V_{\text{H}}(\mathbf{r}),$$

Long range but minor contribution

Screened core-core repulsion energy

$$E_{\text{scc}} = \frac{1}{2} \sum_{I,J} \left[\frac{Z_I Z_J}{|\tau_I - \tau_J|} - \int d\mathbf{r}^3 n_I^{(\text{a})}(\mathbf{r}) V_{\text{H},J}^{(\text{a})}(\mathbf{r}) \right].$$

Short range and two-center integrals

Difference charge

$$\begin{aligned} \delta n(\mathbf{r}) &= n(\mathbf{r}) - n^{(\text{a})}(\mathbf{r}), \\ &= n(\mathbf{r}) - \sum_i n_i^{(\text{a})}(\mathbf{r}), \end{aligned}$$

Neutral atom potential

$$V_{\text{na},I}(\mathbf{r} - \tau_I) = V_{\text{core},I}(\mathbf{r} - \tau_I) + V_{\text{H},I}^{(\text{a})}(\mathbf{r} - \tau_I).$$

Implementation: Total energy (3)

So, the total energy is given by

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{na}} + E_{\text{ec}}^{(\text{NL})} + E_{\delta\text{ee}} + E_{\text{xc}} + E_{\text{scc}}.$$

Each term is evaluated by using a different numerical grid with consideration on accuracy and efficiency.

$$\left. \begin{array}{l} E_{\text{kin}} \\ E_{\text{na}} \\ E_{\text{ec}}^{(\text{NL})} \end{array} \right\} \text{ Spherical coordinate in momentum space}$$

$$\left. \begin{array}{l} E_{\delta\text{ee}} \\ E_{\text{xc}} \end{array} \right\} \text{ Real space regular mesh}$$

$$E_{\text{scc}} \quad \text{Real space fine mesh}$$

Two center integrals

Fourier-transformation of basis functions

$$\begin{aligned}
 \tilde{\phi}_{i\alpha}(\mathbf{k}) &= \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int d\mathbf{r}^3 \phi_{i\alpha}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \\
 &= \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int d\mathbf{r}^3 Y_{lm}(\hat{\mathbf{r}}) R_{pl}(r) \left\{ 4\pi \sum_{L=0}^{\infty} \sum_{M=-L}^L (-i)^L j_L(kr) Y_{LM}(\hat{\mathbf{k}}) Y_{LM}^*(\hat{\mathbf{r}}) \right\}, \\
 &= \left(\frac{1}{\sqrt{2\pi}}\right)^3 4\pi \sum_{L=0}^{\infty} \sum_{M=-L}^L (-i)^L Y_{LM}(\hat{\mathbf{k}}) \int dr r^2 R_{pl}(r) j_L(kr) \int d\theta d\phi \sin(\theta) Y_{lm}(\hat{\mathbf{r}}) Y_{LM}^*(\hat{\mathbf{r}}), \\
 &= \left[\left(\frac{1}{\sqrt{2\pi}}\right)^3 4\pi (-i)^l \int dr r^2 R_{pl}(r) j_L(kr) \right] Y_{lm}(\hat{\mathbf{k}}), \\
 &= \tilde{R}_{pl}(k) Y_{lm}(\hat{\mathbf{k}}),
 \end{aligned}$$

Integrals for angular parts are analytically performed. Thus, we only have to perform one-dimensional integrals along the radial direction.

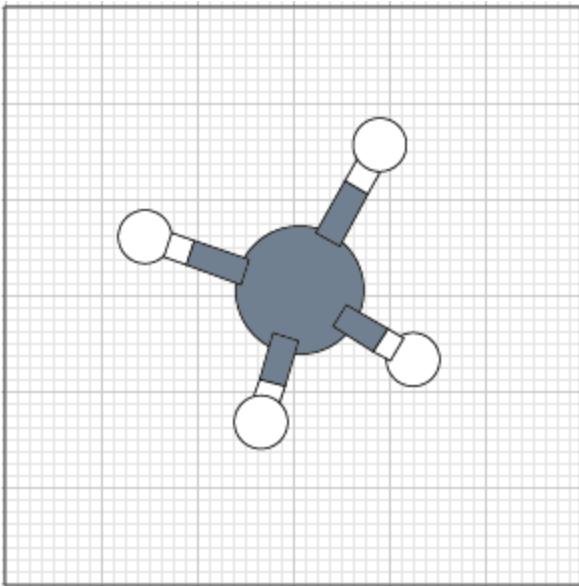
e.g., overlap integral

$$\begin{aligned}
 \langle \phi_{i\alpha}(\mathbf{r}) | \phi_{j\beta}(\mathbf{r} - \tau) \rangle &= \int d\mathbf{r}^3 \phi_{i\alpha}^*(\mathbf{r}) \phi_{j\beta}(\mathbf{r} - \tau), \\
 &= \int d\mathbf{r}^3 \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int dk^3 \tilde{R}_{pl}^*(k) Y_{lm}^*(\hat{\mathbf{k}}) e^{-i\mathbf{k}\cdot\mathbf{r}} \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int dk'^3 \tilde{R}_{p'l'}(k') Y_{l'm'}(\hat{\mathbf{k}}') e^{i\mathbf{k}'\cdot(\mathbf{r}-\tau)}, \\
 &= \left(\frac{1}{2\pi}\right)^3 \int dk^3 \int dk'^3 e^{-i\mathbf{k}'\cdot\tau} \tilde{R}_{pl}^*(k) Y_{lm}^*(\hat{\mathbf{k}}) \tilde{R}_{p'l'}(k') Y_{l'm'}(\hat{\mathbf{k}}') \int d\mathbf{r}^3 e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}, \\
 &= \int dk^3 e^{-i\mathbf{k}\cdot\tau} \tilde{R}_{pl}^*(k) Y_{lm}^*(\hat{\mathbf{k}}) \tilde{R}_{p'l'}(k) Y_{l'm'}(\hat{\mathbf{k}}),
 \end{aligned}$$

Cutoff energy for regular mesh

The two energy components $E_{\delta ee} + E_{xc}$ are calculated on real space regular mesh. The mesh fineness is determined by plane-wave cutoff energies.

```
scf.energycutoff      150.0      # default=150 (Ry)
```



The cutoff energy can be related to the mesh fineness by the following eqs.

$$E_{\text{cut}}^{(1)} = \frac{1}{2} \mathbf{g}\mathbf{b}_1 \cdot \mathbf{g}\mathbf{b}_1, \quad E_{\text{cut}}^{(2)} = \frac{1}{2} \mathbf{g}\mathbf{b}_2 \cdot \mathbf{g}\mathbf{b}_2, \quad E_{\text{cut}}^{(3)} = \frac{1}{2} \mathbf{g}\mathbf{b}_3 \cdot \mathbf{g}\mathbf{b}_3,$$

$$\mathbf{g}\mathbf{a}_1 = \frac{\mathbf{a}_1}{N_1}, \quad \mathbf{g}\mathbf{a}_2 = \frac{\mathbf{a}_2}{N_2}, \quad \mathbf{g}\mathbf{a}_3 = \frac{\mathbf{a}_3}{N_3},$$

$$\mathbf{g}\mathbf{b}_1 = 2\pi \frac{\mathbf{g}\mathbf{a}_2 \times \mathbf{g}\mathbf{a}_3}{\Delta V}, \quad \mathbf{g}\mathbf{b}_2 = 2\pi \frac{\mathbf{g}\mathbf{a}_3 \times \mathbf{g}\mathbf{a}_1}{\Delta V}, \quad \mathbf{g}\mathbf{b}_3 = 2\pi \frac{\mathbf{g}\mathbf{a}_1 \times \mathbf{g}\mathbf{a}_2}{\Delta V},$$

$$\Delta V = \mathbf{g}\mathbf{a}_1 \cdot (\mathbf{g}\mathbf{a}_2 \times \mathbf{g}\mathbf{a}_3),$$

Forces

$$\begin{aligned} \mathbf{F}_i &= -\frac{\partial E_{\text{tot}}}{\partial \mathbf{R}_i} \\ &= -\boxed{\frac{\partial E_{\text{kin}}}{\partial \mathbf{R}_i}} - \boxed{\frac{\partial E_{\text{na}}}{\partial \mathbf{R}_i}} - \boxed{\frac{\partial E_{\text{scc}}}{\partial \mathbf{R}_i}} - \boxed{\frac{\partial E_{\delta\text{ee}}}{\partial \mathbf{R}_i}} - \boxed{\frac{\partial E_{\text{xc}}}{\partial \mathbf{R}_i}} - \boxed{\frac{\partial E_{\text{cc}}}{\partial \mathbf{R}_i}} \end{aligned}$$

$$\frac{\partial E_{\delta\text{ee}}}{\partial \mathbf{R}_k} = \sum_{\mathbf{p}} \frac{\partial n(\mathbf{r}_{\mathbf{p}})}{\partial \mathbf{R}_k} \frac{\partial E_{\delta\text{ee}}}{\partial n(\mathbf{r}_{\mathbf{p}})} + \sum_{\mathbf{p}} \frac{\partial n^{\text{a}}(\mathbf{r}_{\mathbf{p}})}{\partial \mathbf{R}_k} \frac{\partial E_{\delta\text{ee}}}{\partial n^{\text{a}}(\mathbf{r}_{\mathbf{p}})}.$$

$$\begin{aligned} \frac{\partial E_{\delta\text{ee}}}{\partial n(\mathbf{r}_{\mathbf{p}})} &= \frac{1}{2} \Delta V \{ \delta V_{\text{H}}(\mathbf{r}_{\mathbf{p}}) + \sum_{\mathbf{q}} \delta n(\mathbf{r}_{\mathbf{q}}) \frac{\partial \delta V_{\text{H}}(\mathbf{r}_{\mathbf{q}})}{\partial n(\mathbf{r}_{\mathbf{p}})} \}, \\ &= \frac{1}{2} \Delta V \{ \delta V_{\text{H}}(\mathbf{r}_{\mathbf{p}}) + \frac{4\pi}{N_{\text{rsg}}} \sum_{\mathbf{G}} \frac{1}{|\mathbf{G}|^2} \sum_{\mathbf{q}} \delta n(\mathbf{r}_{\mathbf{q}}) e^{i\mathbf{G} \cdot (\mathbf{r}_{\mathbf{q}} - \mathbf{r}_{\mathbf{p}})} \}, \\ &= \Delta V \delta V_{\text{H}}(\mathbf{r}_{\mathbf{p}}). \end{aligned}$$



Easy calc.



See the left

$$\begin{aligned} \frac{\partial E_{\delta\text{ee}}}{\partial n^{\text{a}}(\mathbf{r}_{\mathbf{p}})} &= -\frac{1}{2} \Delta V \{ \delta V_{\text{H}}(\mathbf{r}_{\mathbf{p}}) - \sum_{\mathbf{q}} \delta n(\mathbf{r}_{\mathbf{q}}) \frac{\partial \delta V_{\text{H}}(\mathbf{r}_{\mathbf{q}})}{\partial n^{\text{a}}(\mathbf{r}_{\mathbf{p}})} \}, \\ &= -\frac{1}{2} \Delta V \{ \delta V_{\text{H}}(\mathbf{r}_{\mathbf{p}}) + \frac{4\pi}{N_{\text{rsg}}} \sum_{\mathbf{G}} \frac{1}{|\mathbf{G}|^2} \sum_{\mathbf{q}} \delta n(\mathbf{r}_{\mathbf{q}}) e^{i\mathbf{G} \cdot (\mathbf{r}_{\mathbf{q}} - \mathbf{r}_{\mathbf{p}})} \}, \\ &= -\Delta V \delta V_{\text{H}}(\mathbf{r}_{\mathbf{p}}). \end{aligned}$$

$$\begin{aligned} \frac{\partial n(\mathbf{r}_{\mathbf{p}})}{\partial \mathbf{R}_k} &= \sum_{i\alpha,j\beta} \sum_{\nu} \{ \frac{\partial c_{i\alpha,\nu}^*}{\partial \mathbf{R}_k} c_{j\beta,\nu} \chi_{i\alpha}(\mathbf{r}) \chi_{j\beta}(\mathbf{r}) + c_{i\alpha,\nu}^* \frac{\partial c_{j\beta,\nu}}{\partial \mathbf{R}_k} \chi_{i\alpha}(\mathbf{r}_{\mathbf{p}}) \chi_{j\beta}(\mathbf{r}_{\mathbf{p}}) \} \\ &\quad + 2 \sum_{\alpha,j\beta} \rho_{k\alpha,j\beta} \frac{\partial \chi_{k\alpha}(\mathbf{r}_{\mathbf{p}})}{\partial \mathbf{R}_k} \chi_{j\beta}(\mathbf{r}_{\mathbf{p}}). \end{aligned}$$

$$\begin{aligned} \frac{\partial E_{\text{xc}}}{\partial \mathbf{R}_k} &= \sum_{\mathbf{p}} \frac{\partial n(\mathbf{r}_{\mathbf{p}})}{\partial \mathbf{R}_k} \frac{\partial E_{\text{xc}}}{\partial n(\mathbf{r}_{\mathbf{p}})}, \\ &= \Delta V \sum_{\mathbf{p}} \frac{\partial n(\mathbf{r}_{\mathbf{p}})}{\partial \mathbf{R}_k} v_{\text{xc}}(n(\mathbf{r}_{\mathbf{p}})). \end{aligned}$$

Forces are always analytic at any grid fineness and at zero temperature, even if numerical basis functions and numerical grids.

- Total energy
- **Pseudopotentials**
- Basis functions

Norm-conserving Vanderbilt pseudopotential

I. Morrion, D.M. Bylander, and L. Kleinman, PRB 47, 6728 (1993).

The following non-local operator proposed by Vanderbilt guarantees that scattering properties are reproduced **around multiple reference energies**.

D. Vanderbilt, PRB 41, 7892 (1990).

$$V_{\text{NL}} = \sum_{i,j} B_{ij} |\beta_i\rangle \langle \beta_j|$$

$$|\chi_i\rangle = V_{\text{NL}}^{(i)} |\phi_i\rangle = (\varepsilon_i - T - V_{\text{loc}}) |\phi_i\rangle$$

$$B_{ij} = \langle \phi_i | \chi_j \rangle$$

$$|\beta_i\rangle = \sum_j (B^{-1})_{ji} |\chi_j\rangle$$

If the following generalized norm-conserving condition is fulfilled, the matrix B is Hermitian, resulting in that V_{NL} is also Hermitian.

$$Q_{ij} = \langle \psi_i | \psi_j \rangle_R - \langle \phi_i | \phi_j \rangle_R$$

If $Q=0$, then $B-B^*=0$

$$B_{ij} - B_{ji}^* = (\varepsilon_i - \varepsilon_j) Q_{ij}$$

This is the norm-conserving PP used in OpenMX

Non-local potentials by Vanderbilt

Let's operate the non-local potential on a pseudized wave function:

$$\begin{aligned}
 \hat{v}^{(\text{NL})} |\phi_k^{(\text{PS})}\rangle &= \sum_{ij} |\beta_i\rangle B_{ij} \langle \beta_j | \phi_k^{(\text{PS})} \rangle \\
 &= \sum_{ij} |\beta_i\rangle B_{ij} \sum_{k'} (B^{-1})_{k'j} \langle \chi_{k'} | \phi_k^{(\text{PS})} \rangle, \quad \text{Noting the following relations:} \\
 &= \sum_{ij} |\beta_i\rangle B_{ij} \sum_{k'} (B^{-1})_{k'j} B_{kk'}, \\
 &= \sum_{ij} |\beta_i\rangle B_{ij} \delta_{kj}, \\
 &= \sum_i \left(\sum_j (B^{-1})_{ji} |\chi_j\rangle \right) B_{ik}. \\
 &= \boxed{|\chi_k\rangle}
 \end{aligned}$$

$$v^{(\text{SL})}(r) = v_{\text{L}}(r) + v_{\text{H}}^{(\text{v})}(r) + v_{\text{xc}}^{(\text{v}+\text{pcc})}(r).$$

$$|\chi_i\rangle = \left(\varepsilon_i + \frac{1}{2} \nabla^2 - v^{(\text{SL})}(r) \right) |\phi_i^{(\text{PS})}\rangle,$$

$$B_{ij} = \langle \phi_i^{(\text{PS})} | \chi_j \rangle$$

$$|\beta_i\rangle = \sum_j (B^{-1})_{ji} |\chi_j\rangle.$$

It turns out that the following Schrodinger eq. is hold.

$$\left(-\frac{1}{2} \nabla^2 + v^{(\text{SL})}(r) + \hat{v}^{(\text{NL})} \right) |\phi_i^{(\text{PS})}\rangle = \varepsilon_i |\phi_i^{(\text{PS})}\rangle.$$

Generalized norm-conserving conditions Q_{ij}

In the Vanderbilt pseudopotential, B is given by

$$B_{ij} = \int_0^{r_c} dr P_i^{(\text{PS})}(r) \left(\varepsilon_j + \frac{1}{2} \frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} - v^{(\text{SL})}(r) \right) P_j^{(\text{PS})}(r),$$

$$B_{ji}^* = \int_0^{r_c} dr P_i^{(\text{PS})}(r) \left(\varepsilon_i + \frac{1}{2} \frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} - v^{(\text{SL})}(r) \right) P_j^{(\text{PS})}(r),$$

Thus, we have

$$B_{ij} - B_{ji}^* = (\varepsilon_j - \varepsilon_i) \int_0^{r_c} dr P_i^{(\text{PS})}(r) P_j^{(\text{PS})}(r) + \frac{1}{2} \int_0^{r_c} dr P_i^{(\text{PS})}(r) P_j''^{(\text{PS})}(r) - \frac{1}{2} \int_0^{r_c} dr P_i''^{(\text{PS})}(r) P_j^{(\text{PS})}(r).$$

By integrating by parts, this can be transformed as

$$\begin{aligned} B_{ij} - B_{ji}^* &= (\varepsilon_j - \varepsilon_i) \langle \phi_i^{(\text{PS})} | \phi_j^{(\text{PS})} \rangle_{r_c} + \frac{1}{2} \left[P_i^{(\text{PS})}(r) P_j'^{(\text{PS})}(r) \right]_0^{r_c} - \frac{1}{2} \left[P_i'^{(\text{PS})}(r) P_j^{(\text{PS})}(r) \right]_0^{r_c}, \\ &= (\varepsilon_j - \varepsilon_i) \langle \phi_i^{(\text{PS})} | \phi_j^{(\text{PS})} \rangle_{r_c} + \frac{1}{2} P_i^{(\text{PS})}(r_c) P_j'^{(\text{PS})}(r_c) - \frac{1}{2} P_i'^{(\text{PS})}(r_c) P_j^{(\text{PS})}(r_c). \quad \dots (1) \end{aligned}$$

As well, the similar calculations can be performed for all electron wave functions.

$$0 = (\varepsilon_j - \varepsilon_i) \langle \phi_i^{(\text{AE})} | \phi_j^{(\text{AE})} \rangle_{r_c} + \frac{1}{2} P_i^{(\text{AE})}(r_c) P_j'^{(\text{AE})}(r_c) - \frac{1}{2} P_i'^{(\text{AE})}(r_c) P_j^{(\text{AE})}(r_c). \quad \dots (2)$$

By subtracting (2) from (1), we obtain a relation between B and Q.

$$B_{ij} - B_{ji}^* = (\varepsilon_i - \varepsilon_j) \left(\langle \phi_i^{(\text{AE})} | \phi_j^{(\text{AE})} \rangle_{r_c} - \langle \phi_i^{(\text{PS})} | \phi_j^{(\text{PS})} \rangle_{r_c} \right).$$

Norm-conserving pseudopotential by MBK

I. Morrion, D.M. Bylander, and L. Kleinman, PRB 47, 6728 (1993).

If $Q_{ij} = 0$, the non-local terms can be transformed to a diagonal form.

$$\begin{aligned} V_{\text{NL}} &= \sum_{i,j} B_{ij} |\beta_i\rangle \langle \beta_j|, \\ &= \sum_i \lambda_i |\alpha_i\rangle \langle \alpha_i| \end{aligned}$$

The form is equivalent to that obtained from the Blochl expansion for TM norm-conserving pseudopotentials. Thus, common routines can be utilized for the MBK and TM pseudopotentials, resulting in easiness of the code development.

To satisfy $Q_{ij}=0$, pseudofunctions are now given by

$$\phi_i = \phi_{\text{TM},i} + f_i \quad f_i = \sum_{l=0} c_l \left[r j_l \left(\frac{r}{r_c} u_{li} \right) \right]$$

The coefficients $\{c\}$ are determined by agreement of derivatives and $Q_{ij}=0$. Once a set of $\{c\}$ is determined, χ is given by

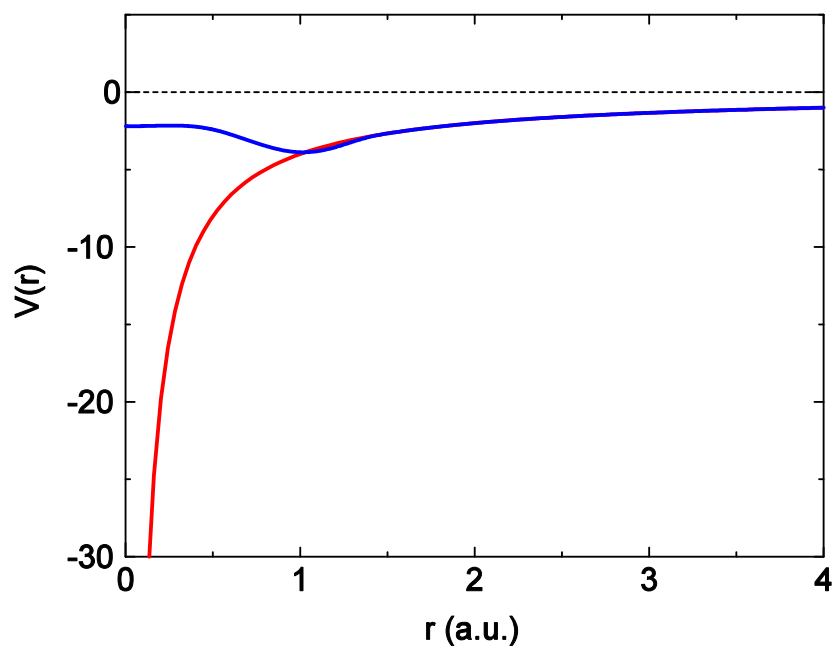
$$\chi_i = V_{\text{TM}}^{(i)} \phi_{\text{TM},i} + \varepsilon_i f_i - V_{\text{loc}} \phi_i - \frac{1}{2} \sum_i c_l \left(\frac{u_{li}}{r_c} \right)^2 \left[r j_l \left(\frac{r}{r_c} u_{li} \right) \right]$$

Pseudo-wave function and pseudopotential of carbon atom

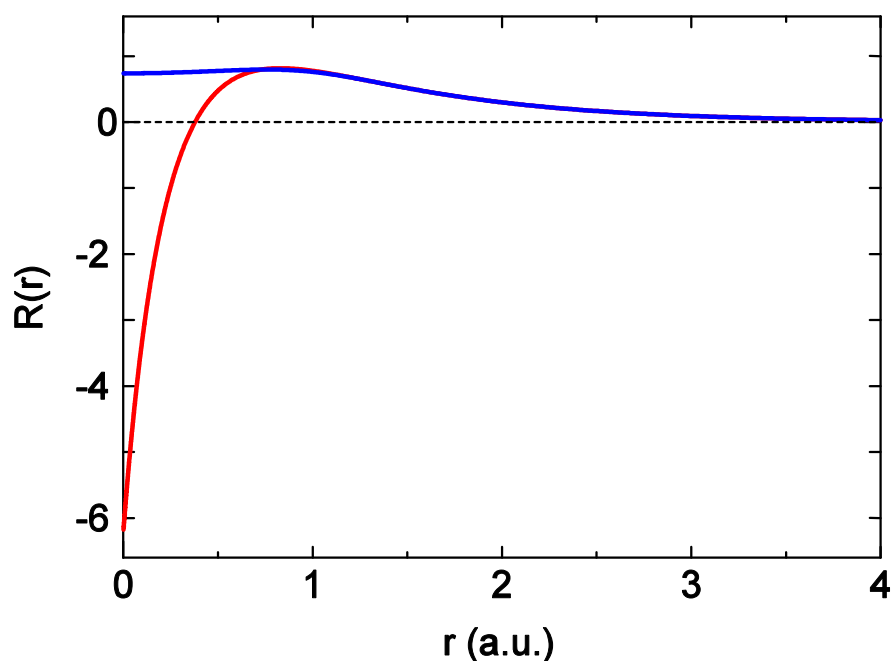
Red: All electron calculation

Blue: Pseudized calculation

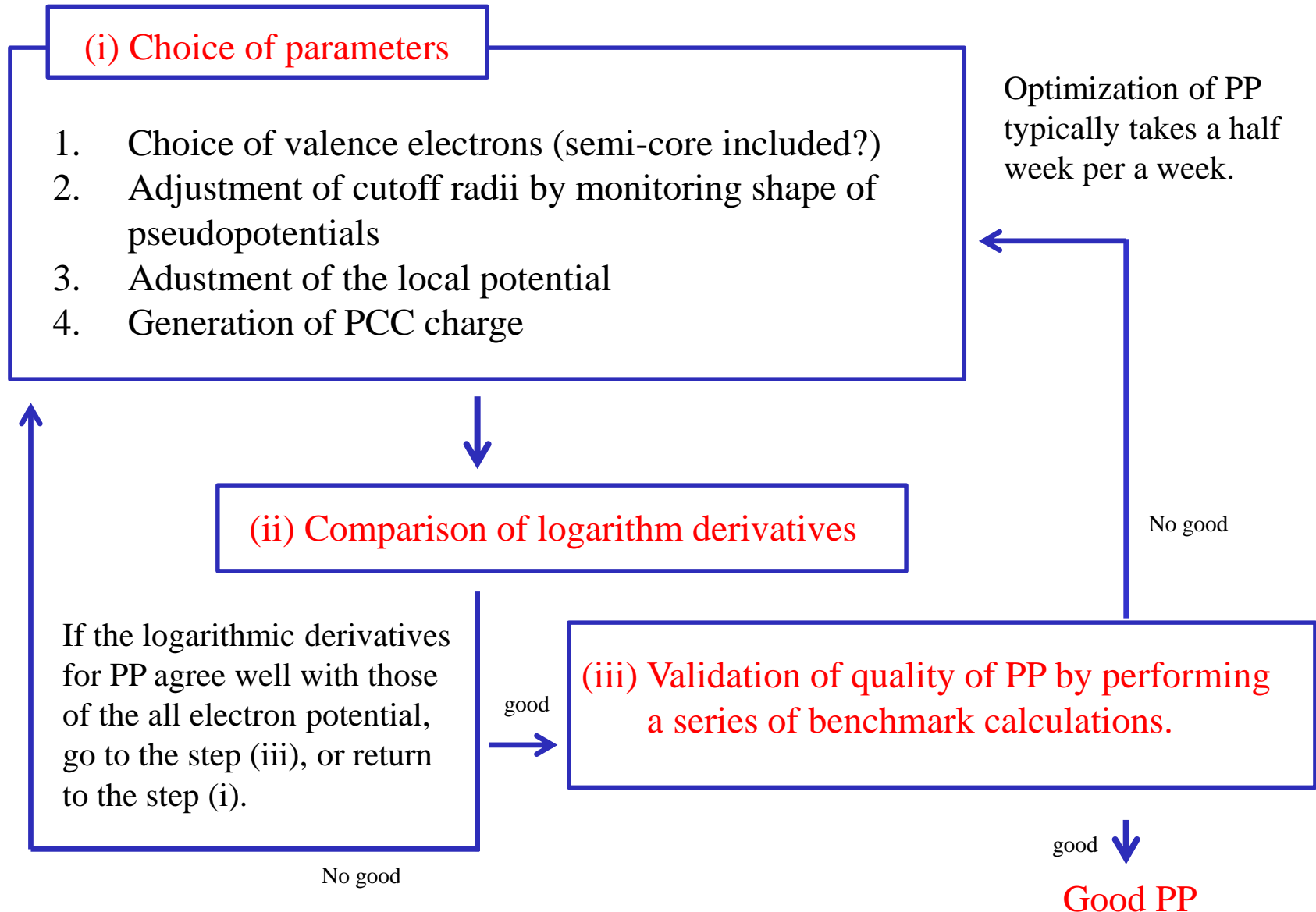
Pseudopotential for C 2s and $-4/r$



Radial wave function of C 2s

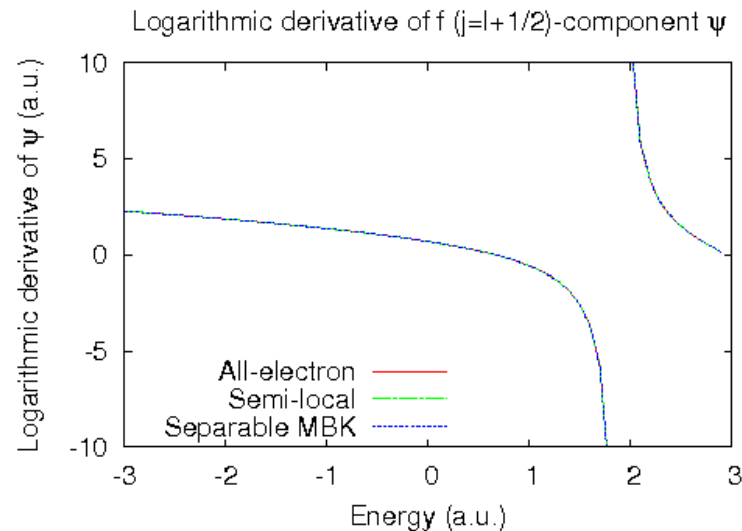
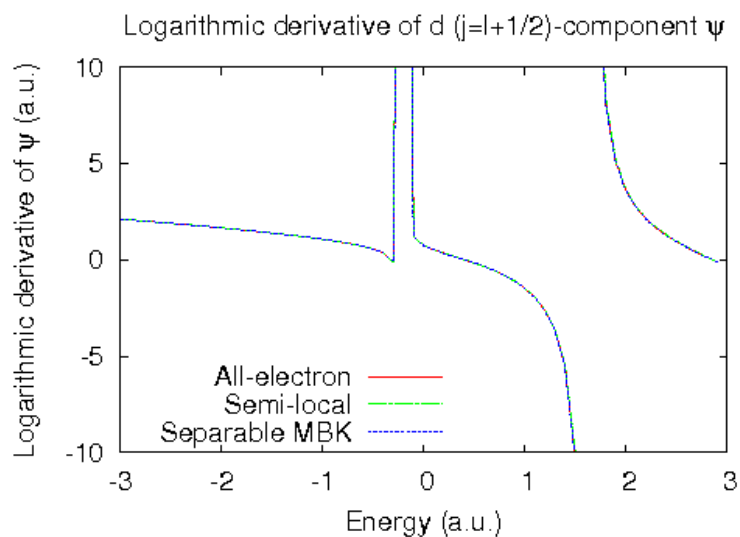
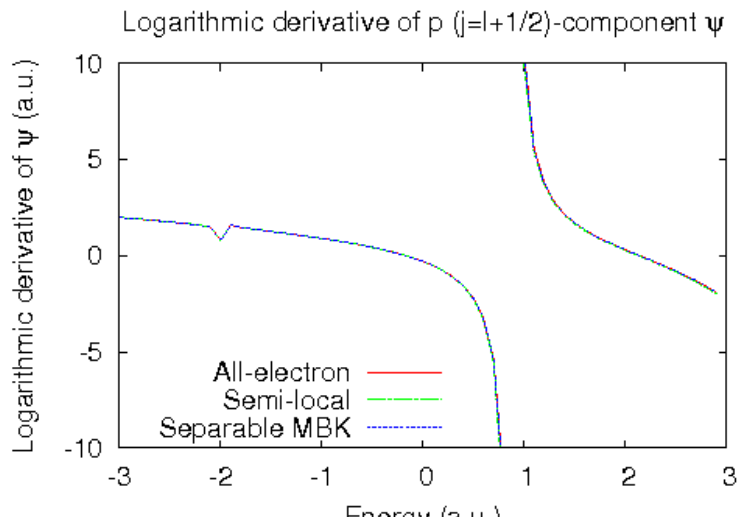
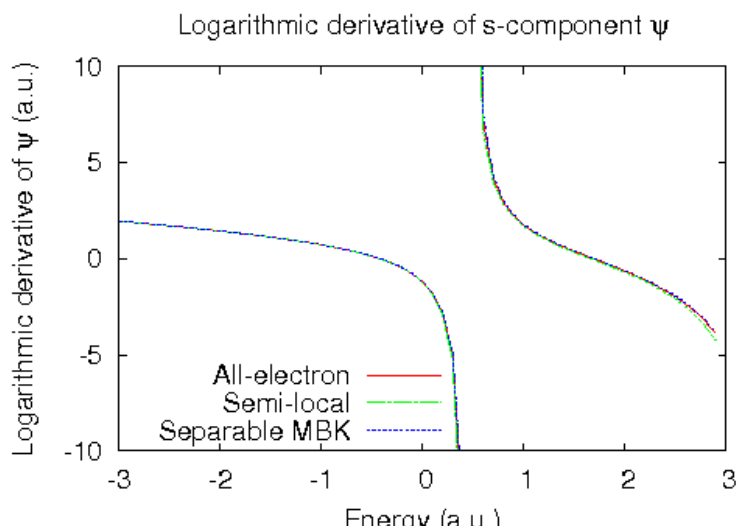


Optimization of pseudopotentials

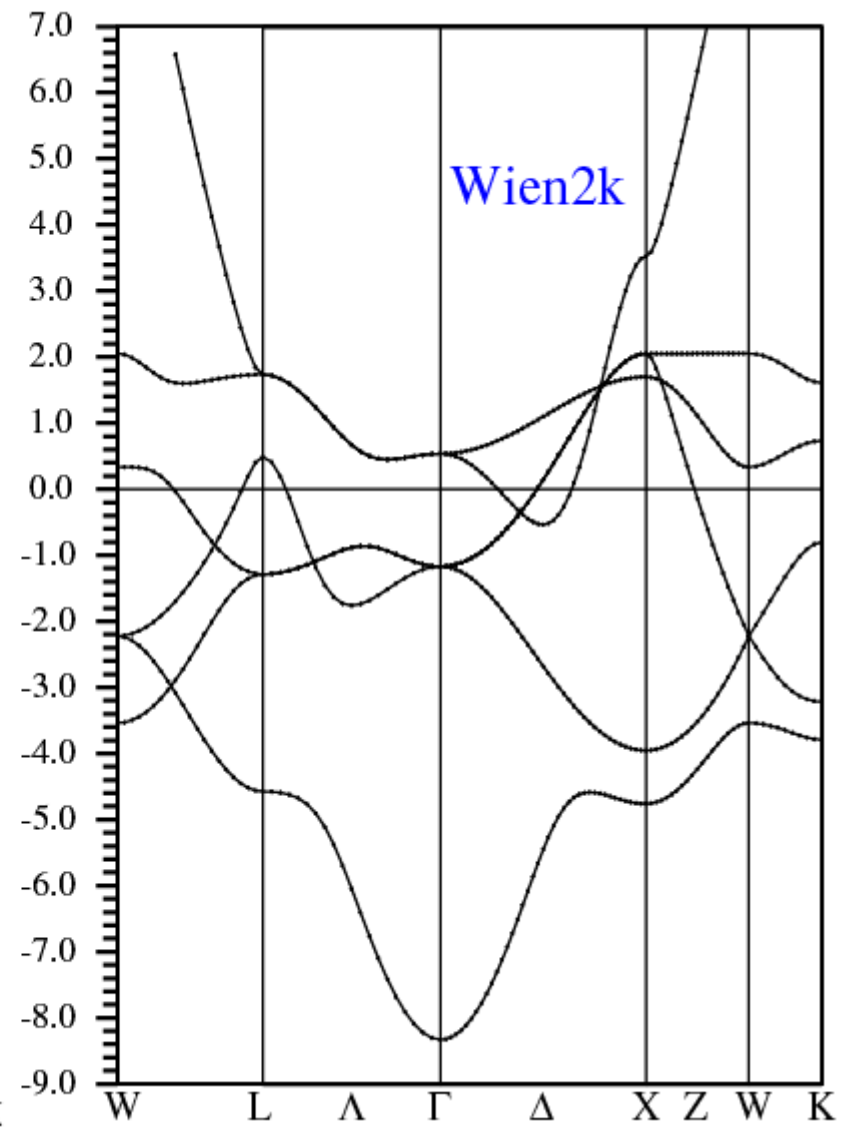
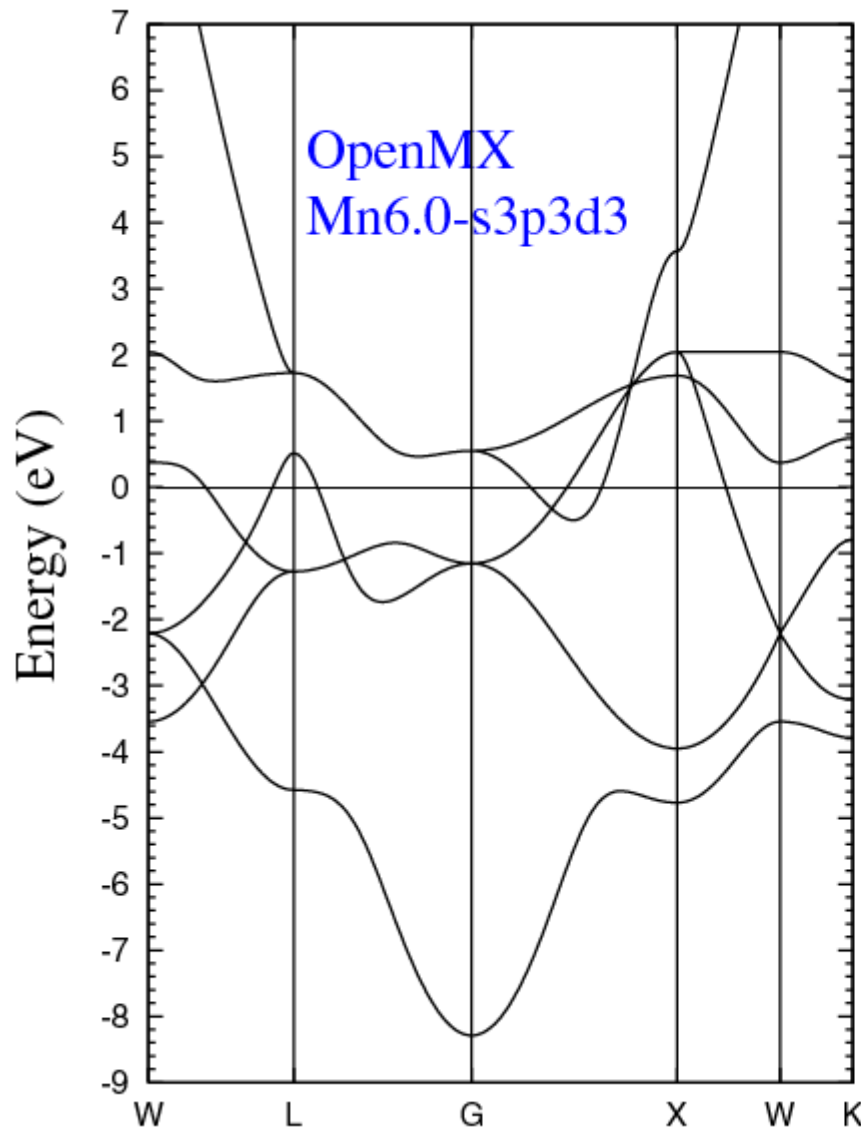


Comparison of logarithmic derivatives

Logarithmic derivatives of s, p, d, f channels for Mn. The deviation between PP and all electron directly affects the band structure.



Comparison of band structure for fcc Mn



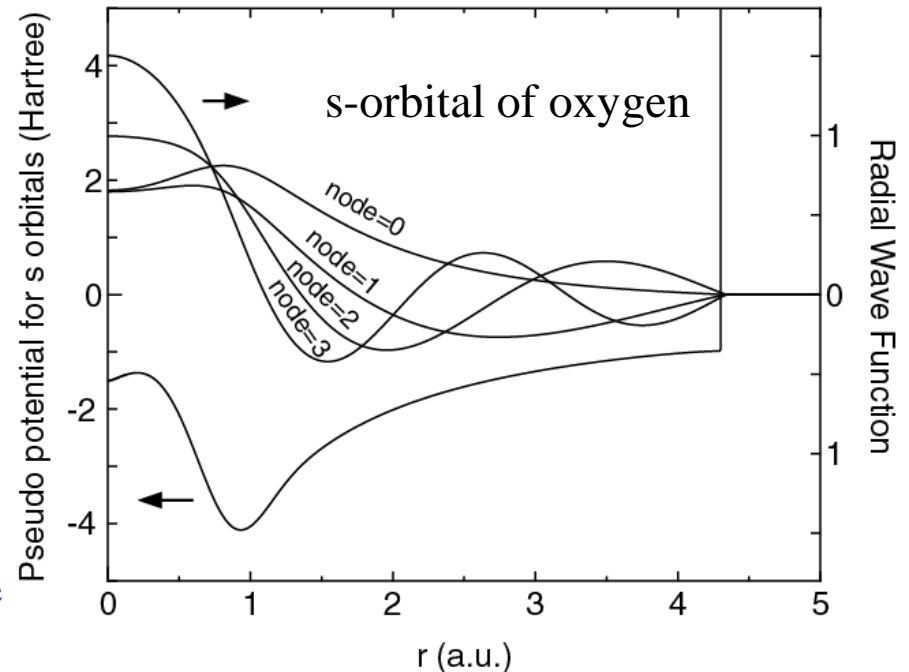
- Total energy
- Pseudopotentials
- **Basis functions**

Primitive basis functions

1. Solve an atomic Kohn-Sham eq. under a confinement potential:

$$V_{\text{core}}(r) = \begin{cases} -\frac{Z}{r} & \text{for } r \leq r_1 \\ \sum_{n=0}^3 b_n r^n & \text{for } r_1 < r \leq r_c \\ h & \text{for } r_c < r, \end{cases}$$

2. Construct the norm-conserving pseudopotentials.
3. Solve ground and excited states for the the pseudopotential for each L-channel.

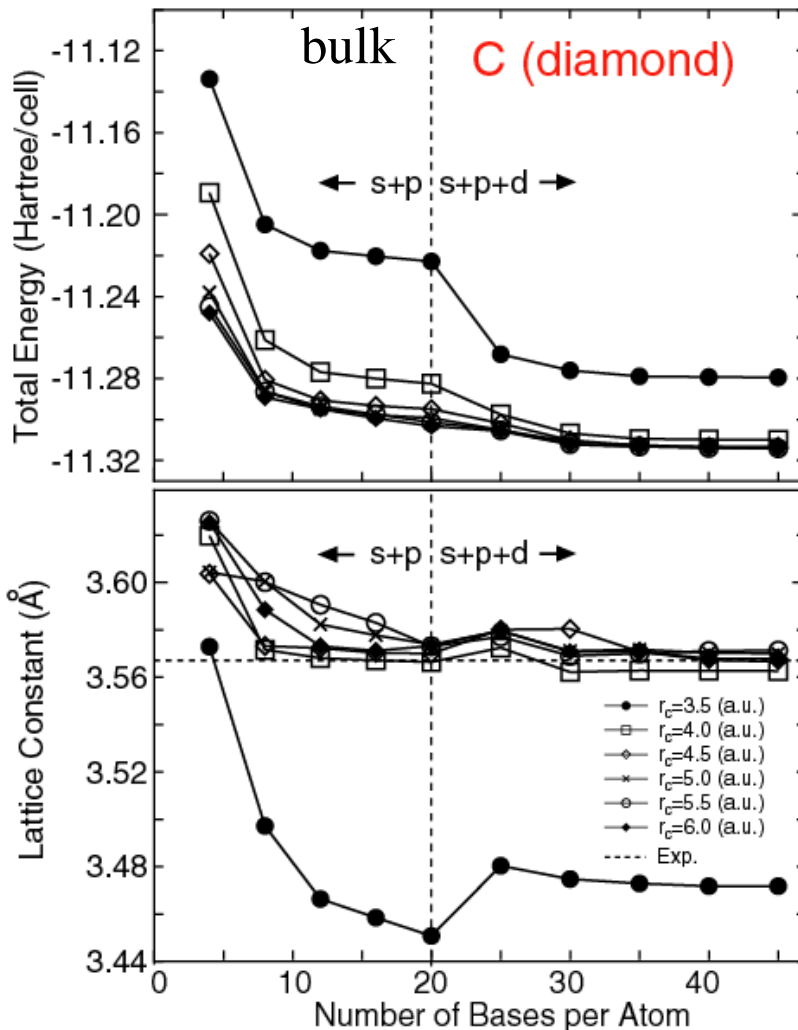
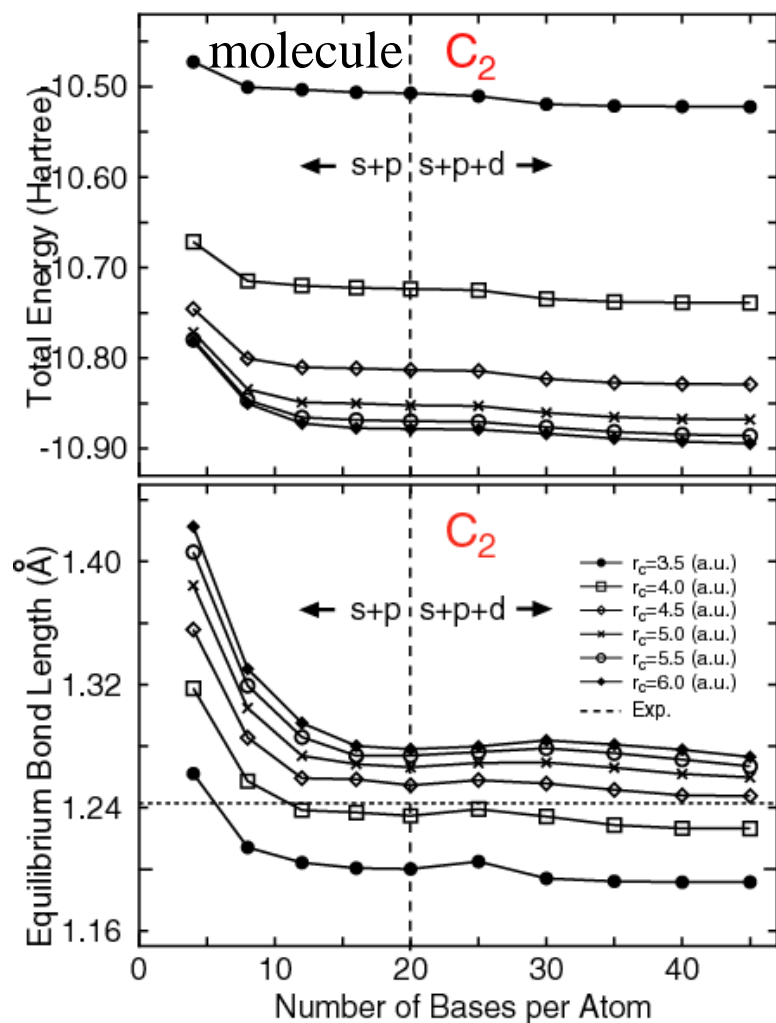


In most cases, the accuracy and efficiency can be controlled by

Cutoff radius
Number of orbitals

Convergence with respect to basis functions

The two parameters can be regarded as variational parameters.



Benchmark of primitive basis functions

Ground state calculations of dimer using primitive basis functions

Dimer	Expt.	Calc.	Dimer	Expt.	Calc.
H ₂ (H4.5- <i>s</i> 2)	$1\Sigma_g^+ a$	$1\Sigma_g^+ (1s\sigma_g^2)$	K ₂ (K10.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (3p\pi_g^4 3p\sigma_u^2 4s\sigma_g^2)$
He ₂ (He7.0- <i>s</i> 2)	$1\Sigma_g^+ b$	$1\Sigma_g^+ (1s\sigma_g^2 1s\sigma_u^2)$	CaO (Ca7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$1\Sigma^+ k$	$1\Sigma^+ (s\sigma^2 s\sigma^2 p\pi^4)$
Li ₂ (Li8.0- <i>s</i> 2)	$1\Sigma_g^+ c$	$1\Sigma_g^+ (2s\sigma_g^2)$	ScO (Sc7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$2\Sigma^+ l$	$2\Sigma^+ (d\pi^4 s\sigma^2 s\sigma^1)$
BeO (Be6.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma^+ d$	$1\Sigma^+ (s\sigma^2 s\sigma^2 p\pi^4)$	Ti ₂ (Ti7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$3\Delta_g m$	$3\Delta_g (4s\sigma_g^2 3d\sigma_g^1 3d\pi_u^4 3d\delta_g^1)$
B ₂ (B5.5- <i>s</i> 2 <i>p</i> 2)	$3\Sigma_g^- e$	$3\Sigma_g^- (2s\sigma_g^2 2s\sigma_u^2 2\pi_u^2)$	V ₂ (V7.5- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$3\Sigma_g^- n$	$1\Sigma_g^+ (4s\sigma_g^2 3d\sigma_g^2 3d\pi_u^4 3d\delta_g^2)$
C ₂ (C5.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (2s\sigma_g^2 2s\sigma_u^2 2p\pi_u^4)$	V ₂ (V7.5- <i>s</i> 4 <i>p</i> 4 <i>d</i> 4 <i>f</i> 2)	$3\Sigma_g^- n$	$3\Sigma_g^- (4s\sigma_g^2 3d\sigma_g^2 3d\pi_u^4 3d\delta_g^2)$
N ₂ (N5.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (2s\sigma_u^2 2p\pi_u^4 2p\sigma_g^2)$	Cr ₂ (Cr7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$1\Sigma^+ o$	$1\Sigma^+ (4s\sigma_g^2 3d\sigma_g^2 3d\pi_u^4 3d\delta_g^4)$
O ₂ (O5.0- <i>s</i> 2 <i>p</i> 2)	$3\Sigma_g^- f$	$3\Sigma_g^- (2p\sigma_g^2 2p\pi_u^4 2p\pi_g^2)$	MnO (Mn7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$6\Sigma^+ p$	$6\Sigma^+ (d\sigma^1 d\pi^4 d\delta^2 d\pi^{*2})$
F ₂ (F5.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (2p\sigma_g^2 2p\pi_u^4 2p\pi_g^4)$	Fe ₂ (Fe7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$7\Delta_u q$	$7\Delta_u (4s\sigma_g^2 3d\sigma_g^2 3d\sigma_u^1 3d\pi_u^4 3d\pi_g^2 3d\delta_g^3 3d\delta_u^2)$
Ne ₂ (Ne7.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ g$	$1\Sigma_g^+ (2p\pi_u^4 2p\pi_g^4 2p\sigma_u^2)$	Co ₂ (Co7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)		$5\Delta_g (4s\sigma_g^2 3d\sigma_g^2 3d\sigma_u^1 3d\pi_u^4 3d\pi_g^2 3d\delta_g^4 3d\delta_u^3)$
Na ₂ (Na9.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (2p\pi_g^4 2p\sigma_u^2 3s\sigma_g^2)$	Ni ₂ (Ni7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	Ωr	$3\Sigma_g^- (4s\sigma_g^2 3d\sigma_g^2 3d\sigma_u^2 3d\pi_u^4 3d\pi_g^2 3d\delta_g^4 3d\delta_u^4)$
MgO (Mg7.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma^+ h$	$1\Sigma^+ (s\sigma^2 s\sigma^2 p\pi^4)$	Cu ₂ (Cu7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$1\Sigma_g^+ s$	$1\Sigma_g^+ (4s\sigma_g^2 3d\sigma_g^2 3d\sigma_u^2 3d\pi_u^4 3d\pi_g^4 3d\delta_g^4 3d\delta_u^4)$
Al ₂ (Al6.5- <i>s</i> 2 <i>p</i> 2)	$3\Pi_u i$	$3\Sigma_g^- (3s\sigma_g^2 3s\sigma_u^2 3p\pi_u^2)$	ZnH (Zn7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$2\Sigma_g^+ t$	$2\Sigma_g^+ (s\sigma^2 s\sigma^{*1} d\sigma^2 d\pi^4 d\delta^4)$
Al ₂ (Al6.5- <i>s</i> 4 <i>p</i> 4 <i>d</i> 2)	$3\Pi_u i$	$3\Sigma_g^- (3s\sigma_g^2 3s\sigma_u^2 3p\pi_u^2)$	GaH (Ga7.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma^+ u$	$1\Sigma^+ (s\sigma^2 s\sigma^{*2})$
Si ₂ (Si6.5- <i>s</i> 2 <i>p</i> 2)	$3\Sigma_g^- f$	$3\Pi_u (3s\sigma_u^2 3s\sigma_g^1 3p\pi_u^3)$	GeO (Ge7.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma^+ f$	$1\Sigma^+ (ss\sigma^2 sp\sigma^2 pp\pi^4 pp\sigma^2)$
Si ₂ (Si6.5- <i>s</i> 2 <i>p</i> 2 <i>d</i> 1)	$3\Sigma_g^- f$	$3\Sigma_g^- (3s\sigma_u^2 3p\pi_u^2 3s\sigma_g^2)$	As ₂ (As7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 1)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (4s\sigma_g^2 4s\sigma_u^2 4p\sigma_g^2 4p\pi_u^4)$
P ₂ (P6.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 1)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (3s\sigma_u^2 3p\sigma_g^2 3p\pi_u^4)$	Se ₂ (Se7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 1)	$3\Sigma_g^- f$	$3\Sigma_g^- (4s\sigma_g^2 4s\sigma_u^2 4p\sigma_g^2 4p\pi_u^4 4p\pi_g^2)$
S ₂ (S6.0- <i>s</i> 2 <i>p</i> 2)	$3\Sigma_g^- f$	$3\Sigma_g^- (3p\sigma_g^2 3p\pi_u^4 3p\pi_g^2)$	Br ₂ (Br7.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 1)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (4s\sigma_g^2 4s\sigma_u^2 4p\sigma_g^2 4p\pi_u^4 4p\pi_g^4)$
Cl ₂ (Cl6.0- <i>s</i> 2 <i>p</i> 2 <i>d</i> 2)	$1\Sigma_g^+ f$	$1\Sigma_g^+ (3p\sigma_g^2 3p\pi_u^4 3p\pi_g^4)$	Kr ₂ (Kr7.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ v$	$1\Sigma_g^+ (4s\sigma_g^2 4s\sigma_u^2 4p\sigma_g^2 4p\sigma_u^2 4p\pi_u^4 4p\pi_g^4)$
Ar ₂ (Ar7.0- <i>s</i> 2 <i>p</i> 2)	$1\Sigma_g^+ j$	$1\Sigma_g^+ (3p\pi_u^4 3p\pi_g^4 3p\sigma_u^2)$			

All the successes and failures by the LDA are reproduced by the modest size of basis functions (DNP in most cases)

Variational optimization of basis functions

One-particle wave functions

$$\psi_{\mu}(\mathbf{r}) = \sum_{i\alpha} c_{\mu,i\alpha} \phi_{i\alpha}(\mathbf{r} - \mathbf{r}_i)$$

Contracted orbitals

$$\phi_{i\alpha}(\mathbf{r}) = \sum_q a_{i\alpha q} \chi_{i\eta}(\mathbf{r})$$

The variation of E with respect to c with fixed a gives

$$\partial E_{\text{tot}} / \partial c_{\mu,i\alpha} = 0 \quad \rightarrow \quad \sum_{j\beta} \langle \phi_{i\alpha} | \hat{H} | \phi_{j\beta} \rangle c_{\mu,j\beta} = \varepsilon_{\mu} \sum_{j\beta} \langle \phi_{i\alpha} | \phi_{j\beta} \rangle c_{\mu,j\beta}$$

Regarding c as dependent variables on a and assuming KS eq. is solved self-consistently with respect to c , we have

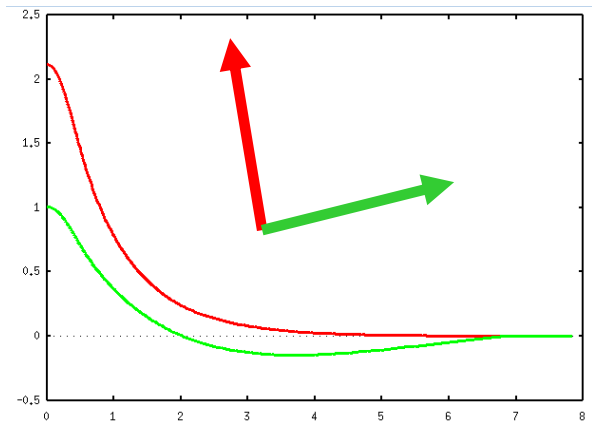
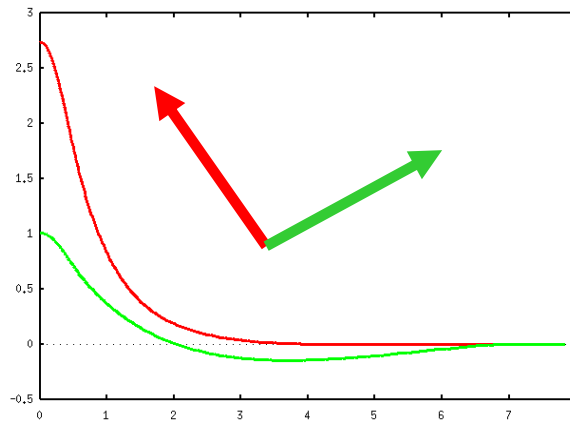
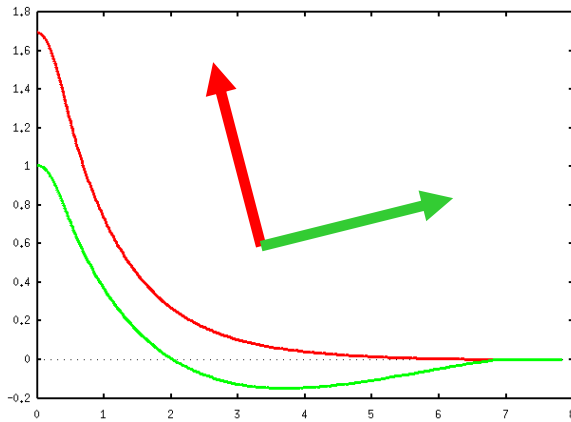
$$\begin{aligned} \frac{\partial E_{\text{tot}}}{\partial a_{i\alpha q}} &= \frac{\delta E_{\text{tot}}}{\delta \rho(\mathbf{r})} \frac{\delta \rho(\mathbf{r})}{\delta a_{i\alpha q}} \\ &= 2 \sum_{j\beta} (\Theta_{i\alpha,j\beta} \langle \chi_{i\eta} | \hat{H} | \phi_{j\beta} \rangle - E_{i\alpha,j\beta} \langle \chi_{i\eta} | \phi_{j\beta} \rangle) \end{aligned}$$

Optimization of basis functions

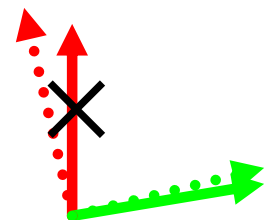
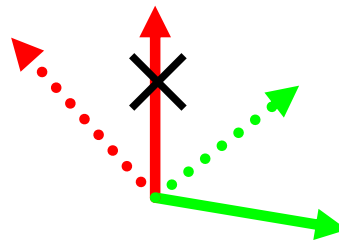
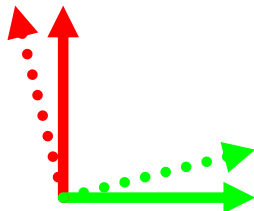
1. Choose typical chemical environments



2. Optimize variationally the radial functions



3. Rotate a set of optimized orbitals within the subspace, and discard the redundant functions



Database of optimized VPS and PAO

Database (2013) of optimized VPS and PAO

The database (2013) of fully relativistic pseudopotentials (VPS) and pseudo-atomic orbitals (PAO), generated by ADPACK, which could be an input data of program package, OpenMX. The data of elements with the underline are currently available. When you use these data, VPS and PAO, in the program package, OpenMX, then copy them to the directory, openmx*/DFT_DATA13/VPS/ and openmx*/DFT_DATA13/PAO/, respectively. The delta factor of OpenMX with the database (2013) is found at [here](#).

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

Reproducibility in DFT calcs

RESEARCH ARTICLE

Science 351, aad3000 (2016)

DFT METHODS

Reproducibility in density functional theory calculations of solids

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15 codes

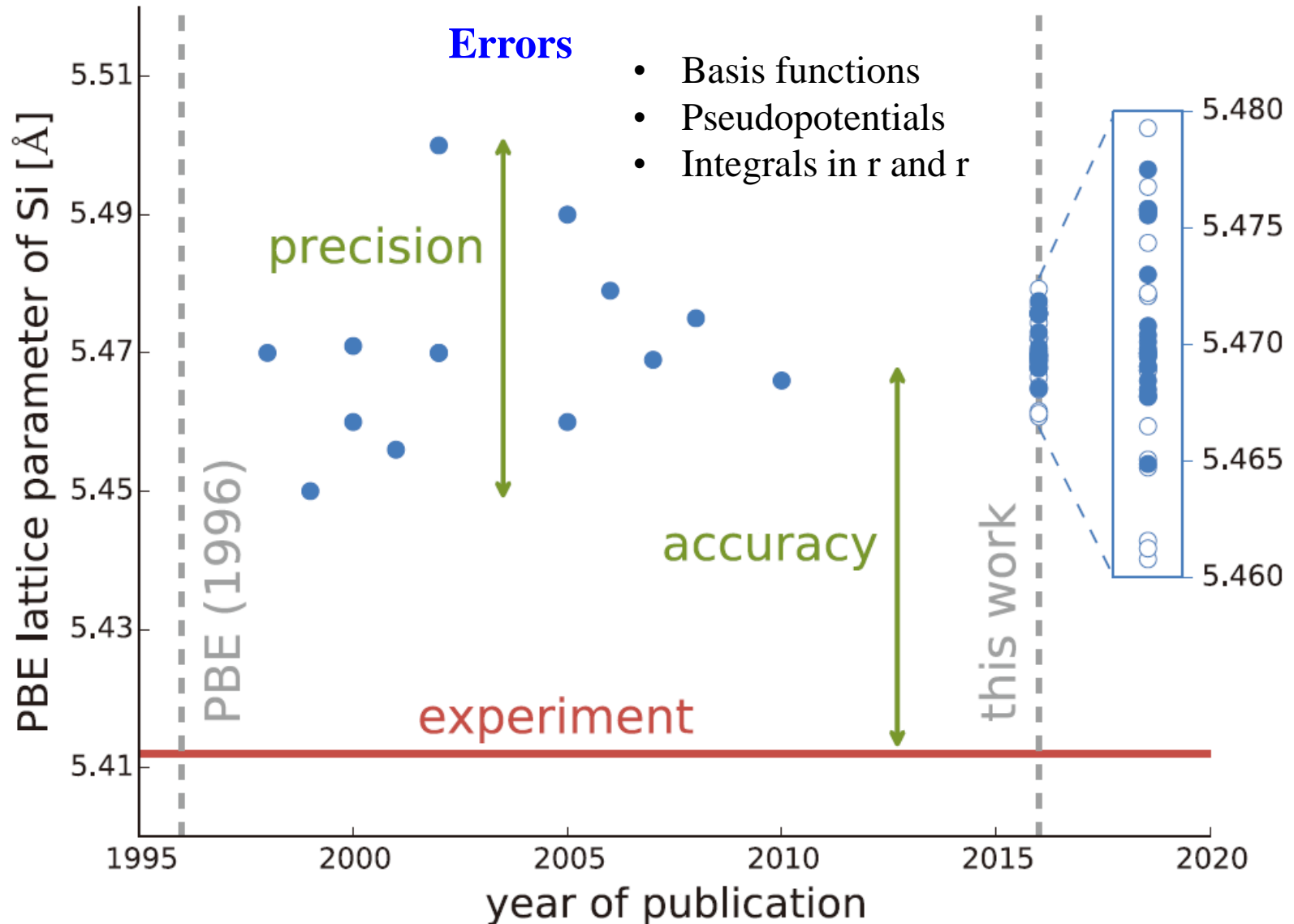
69 researchers

71 elemental bulks

GGA-PBE

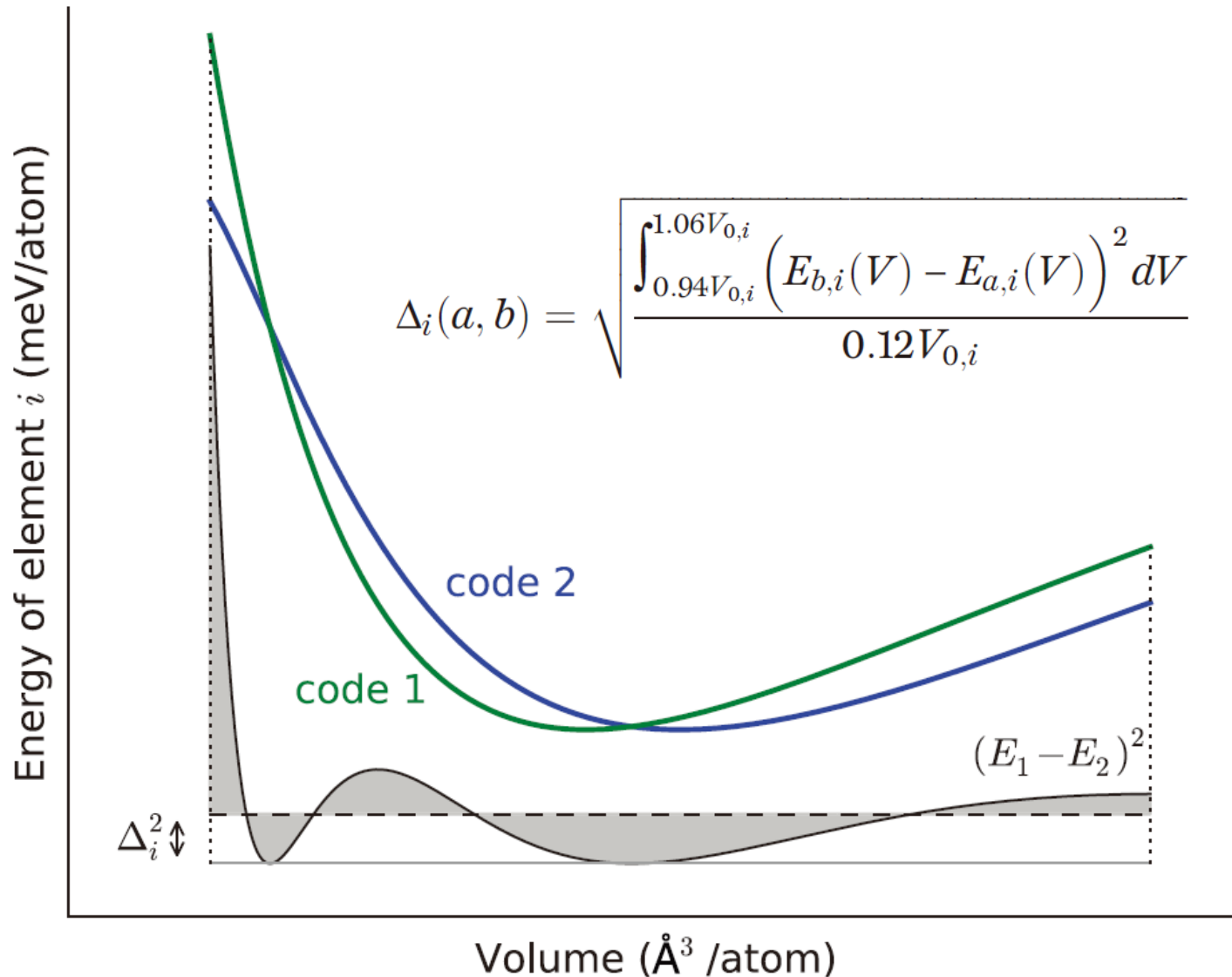
Scalar relativistic

PBE lattice constant of Si



Δ -gauge

A way of comparing accuracy of codes



Evaluation of GGA-PBE By Δ -gauge

In comparison of GGA-PBE with Expts. of 58 elements, the mean Δ -gauge is 23.5meV/atom.

H																	He	
$\Delta(\text{exp}) = 23.5 \text{ meV/atom}$																		
Li	Be											B	C	N	O	F	Ne	
0.4													17.6					17.1
Na	Mg											Al	Si	P	S	Cl	Ar	
0.2	1.5											3.9	13.7	19.0	44.0	46.1	38.6	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
1.4	3.0	1.7	3.0	13.1	1.6	47.7	10.6	3.3	6.2	13.5	7.6		28.2	17.1	11.1	22.3	54.6	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
1.3	2.4	0.7	8.2	14.8	26.5		30.4	44.6	49.1	39.3	34.0	23.6	40.7	25.1	9.9	68.1	59.8	
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
4.0	2.5		2.8	16.8	35.6	29.9	65.2	50.7	54.9	64.0		42.4	32.9	32.0				

$\Delta(\text{exp}) = 23.5 \text{ meV/atom}$

Comparison of codes by Δ -gauge

		AE							
		average $\langle \Delta \rangle$	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	
	GBRV12/ABINIT	0.9	0.9	0.8	0.8	0.9	1.3	1.1	0.8
	GPW09/ABINIT	1.4	1.3	1.3	1.3	1.3	1.7	1.5	1.3
	GPW09/GPAW	1.6	1.5	1.5	1.5	1.5	1.8	1.7	1.5
PAW	JTH02/ABINIT	0.6	0.6	0.6	0.6	0.6	0.9	0.7	0.5
	PS1b100/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
	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
USPP	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
	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
NCP	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

The mean Δ -gauge of OpenMX is 2.0meV/atom.

Summary

- OpenMX is a program package, supporting DFT within LDA, GGA, and plus U, under GNU-GPL.
- The basic strategy to realize large-scale calculations relies on the use of pseudopotentials (PPs) and localized pseudoatomic orbital (PAO) basis functions.
- The careful evaluation of the total energy and optimization of PPs and PAOs guarantee accurate and fast DFT calculations in a balanced way.
- The Δ -gauge might become a standard measure to check accuracy of newly developed codes and functionals.