

Localized basis methods

Theory and implementations

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

Taisuke Ozaki (ISSP, Univ. of Tokyo)

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.

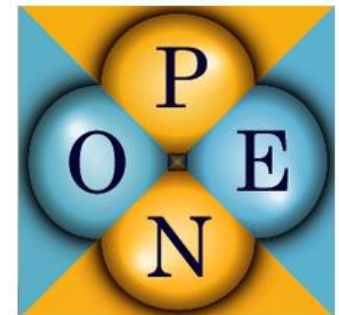
History of OpenMX

- 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

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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)
- [What is OpenMX?](#)
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<http://www.openmx-square.org>

About 400 papers published using OpenMX

Developers of OpenMX

- T. Ozaki (U.Tokyo)
- H. Kino (NIMS)
- J. Yu (SNU)
- M. J. Han (KAIST)
- M. Ohfuti (Fujitsu)
- T. Ohwaki (Nissan)
- H. Weng (CAS)
- M. Toyoda (Osaka Univ.)
- H. Kim (SNU)
- P. Pou (UAM)
- R. Perez (UAM)
- M. Ellner (UAM)
- T. V. Truong Duy (U.Tokyo)
- C.-C. Lee (Univ. of Tokyo))
- Y. Okuno (Fuji FILM)
- Yang Xiao (NUAA)
- F. Ishii (Kanazawa Univ.)
- K. Sawada (RIKEN)
- Y. Kubota (Kanazawa Univ.)
- 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)

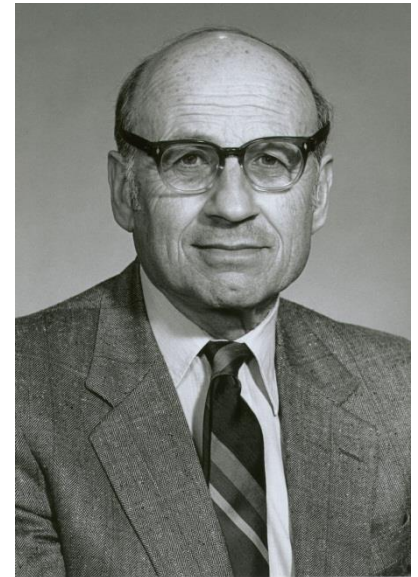
$$E[\rho] = \int \rho(\mathbf{r})v(\mathbf{r})d + T[\rho] + J[\rho] + E_{xc}[\rho]$$

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

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

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

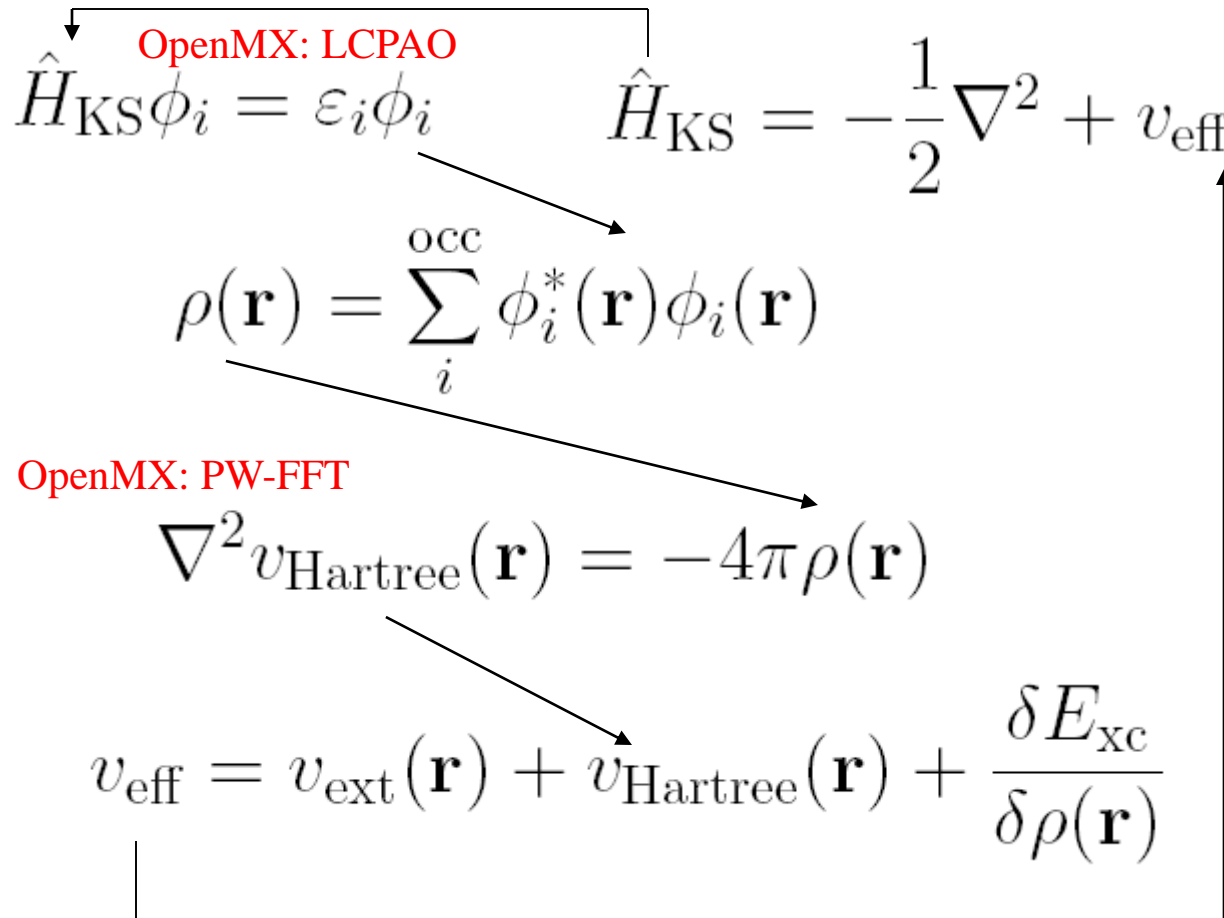
$$v_{\text{eff}} = v_{\text{ext}}(\mathbf{r}) + v_{\text{Hartree}}(\mathbf{r}) + \frac{\delta E_{xc}}{\delta \rho(\mathbf{r})}$$



W.Kohn (1923-)

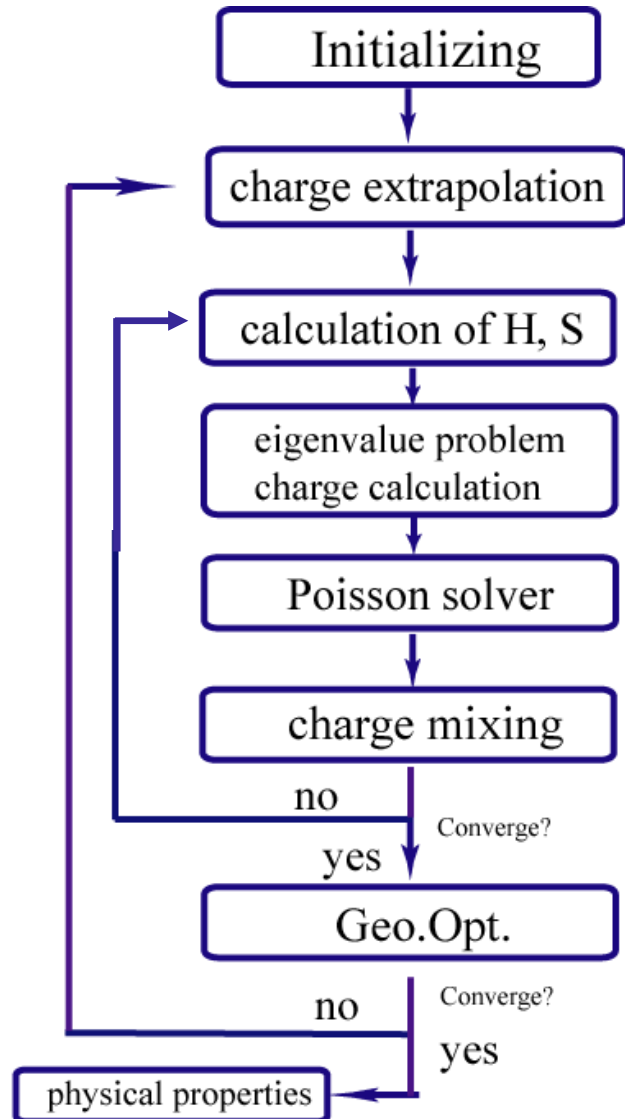
Mathematical structure of KS eq.

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



Input charge = Output charge \rightarrow Self-consistent condition

Flowchart of calculation



The DFT calculations basically consist of two loops. The inner loop is for SCF, and the outer loop is for geometry optimization.

The inner loop may have routines for construction of the KS matrix, eigenvalue problem, solution of Poisson eq., and charge mixing.

After getting a convergent structure, several physical quantities will be calculated.

Classification of the KS solvers

Treatment of core
electrons

All electron (AE) method

Pseudo-potential (PP) method

Basis functions

Plane wave basis (PW)

Mixed basis (MB)

Local basis (LB)

Accuracy

Efficiency

AE+MB: LAPW, LMTO

⊙

×

AE+LB: Gaussian

○

○

PP+PW: Plane wave with PP

○

○

PP+LB: OpenMX, SIESTA

△

⊙

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
- Self-consistency

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.

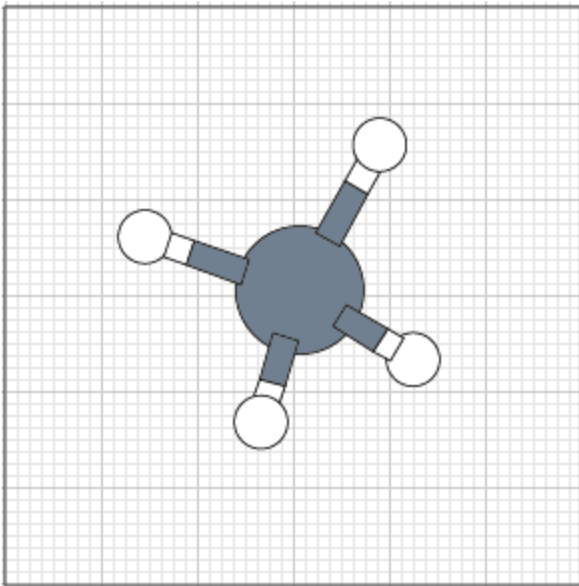
e.g., overlap integral

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

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
- Self-consistency

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

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.

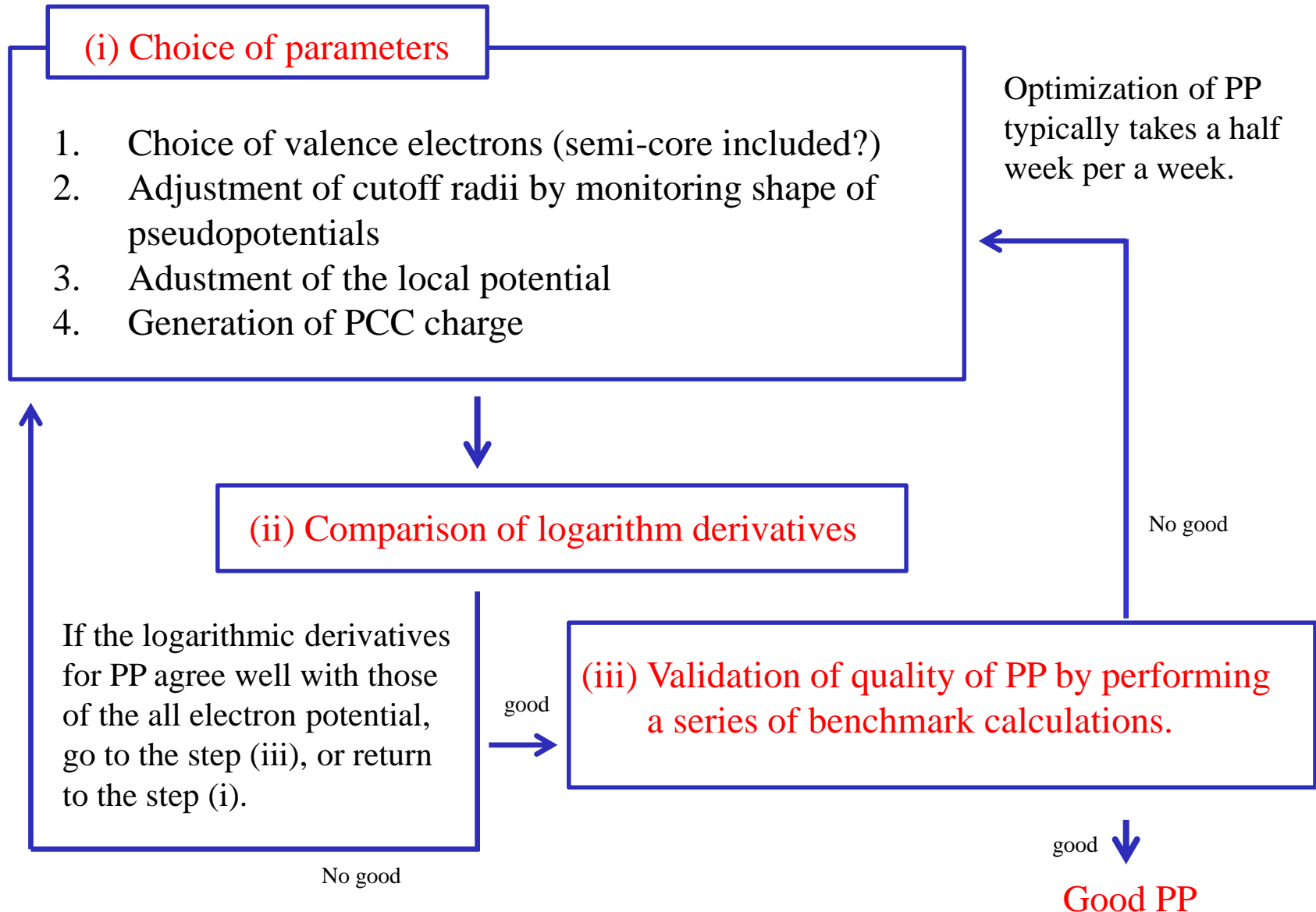
To satisfy $Q_{ij}=0$, pseudofunctions are now given by

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

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

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

Optimization of pseudopotentials



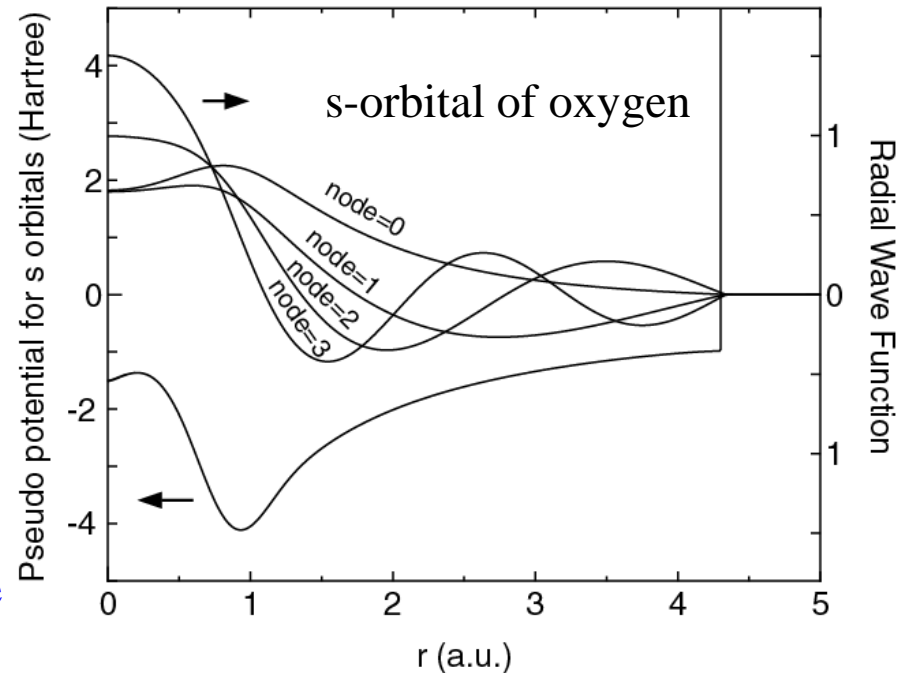
- Total energy
- Pseudopotentials
- **Basis functions**
- Self-consistency

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.

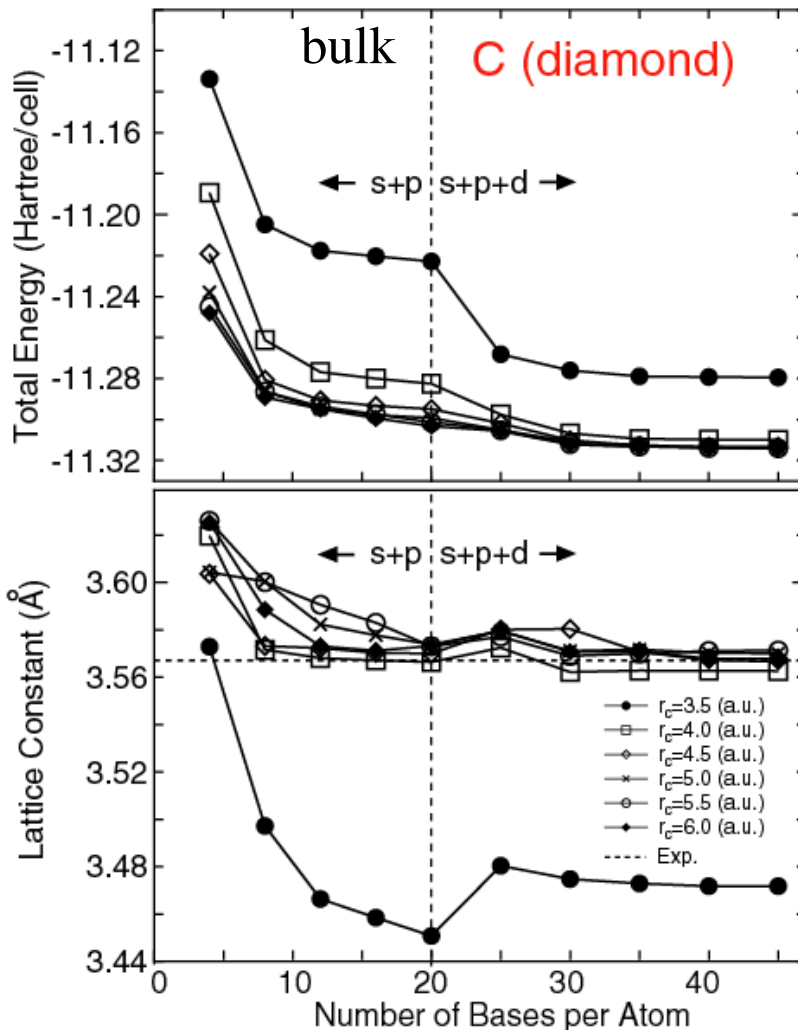
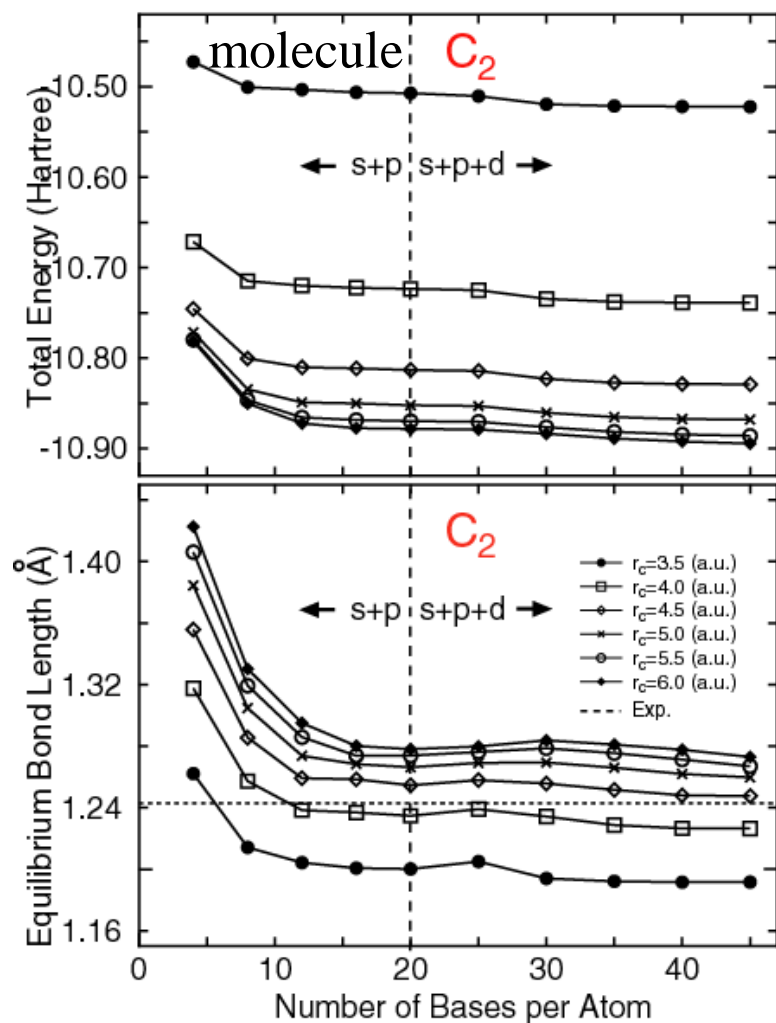


In most cases, the accuracy and efficiency can be controlled by

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)	$2\Sigma^+ t$	$2\Sigma^+ (s\sigma^2 s\sigma^{*1} d\sigma^2 d\pi^4 d\delta^4)$
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

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

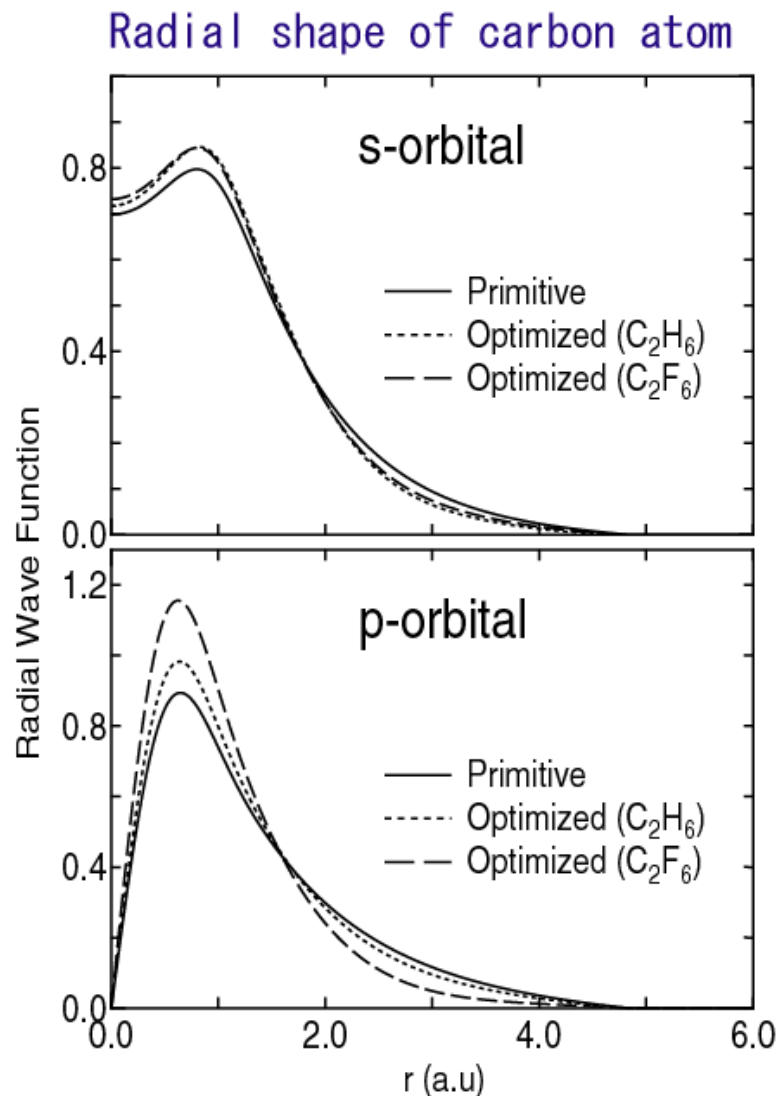
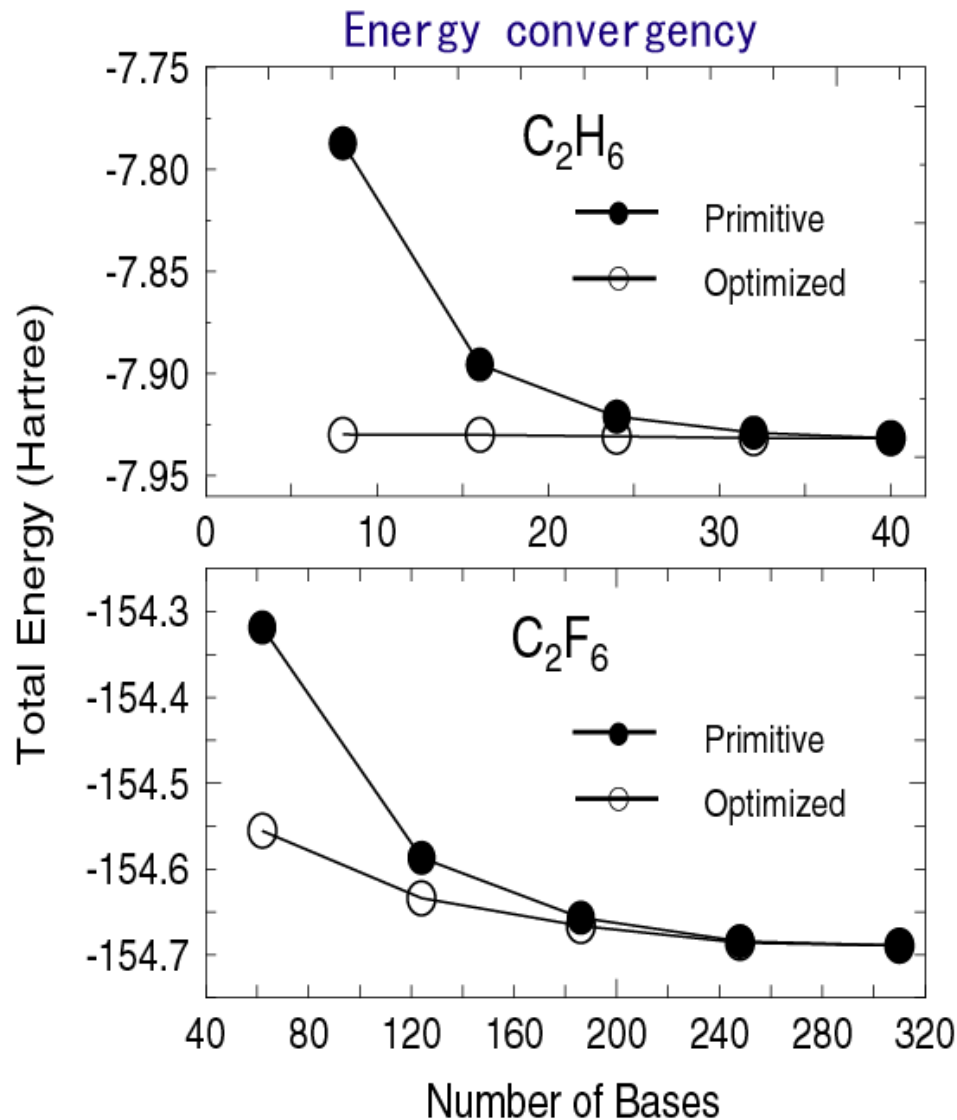
The variation of E with respect to c with fixed a gives

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

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

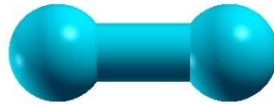
$$\begin{aligned} \frac{\partial E_{\text{tot}}}{\partial a_{i\alpha q}} &= \frac{\delta E_{\text{tot}}}{\delta \rho(\mathbf{r})} \frac{\delta \rho(\mathbf{r})}{\delta a_{i\alpha q}} \\ &= 2 \sum_{j\beta} (\Theta_{i\alpha,j\beta} \langle \chi_{i\eta} | \hat{H} | \phi_{j\beta} \rangle - E_{i\alpha,j\beta}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

Comparison between primitive and optimized basis functions

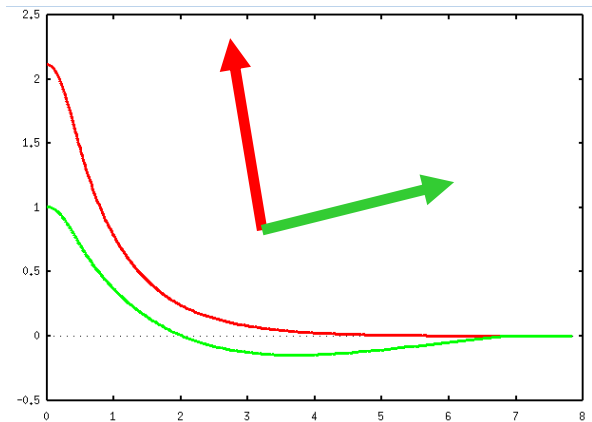
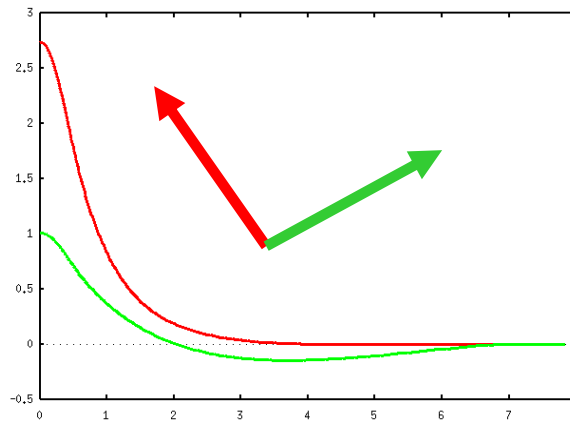
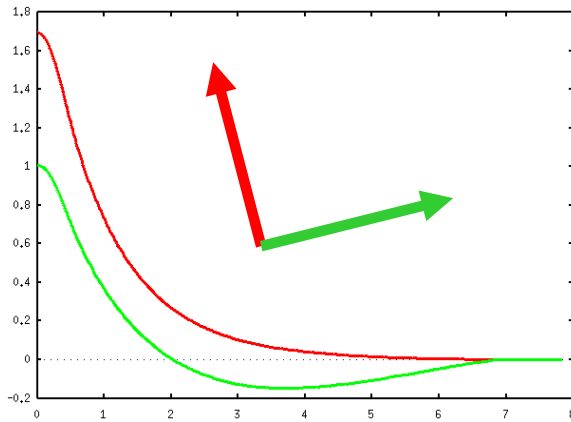


Optimization of basis functions

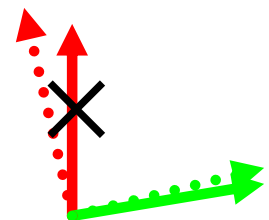
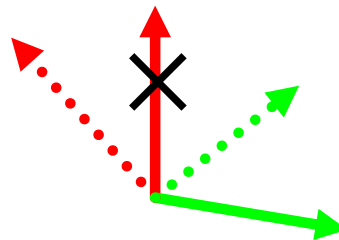
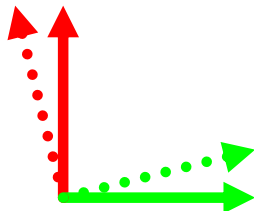
1. Choose typical chemical environments



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.																			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			

- Total energy
- Pseudopotentials
- Basis functions
- **Self-consistency**

Self-consistency: Simple charge mixing

The KS effective is constructed from ρ .

However, ρ is evaluated from eigenfaunctions of KS eq.

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

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

$$\rho(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r})\phi_i(\mathbf{r})$$

Simple charge mixing method

The next input density is constructed by a simple mixing of input and output densities.

$$\rho_{n+1}^{(\text{in})} = \alpha \rho_n^{(\text{in})} + (1 - \alpha) \rho_n^{(\text{out})},$$

It works well for large gap systems and small sized systems.

Self-consistency: RMM-DIIS

Idea:

Minimize the norm of a linear combination of previous residual vectors.

$$\bar{R}_{n+1} = \sum_{m=n-(p-1)}^n \alpha_m R_m,$$

$$R_n(\mathbf{q}) \equiv \tilde{n}_n^{(\text{out})}(\mathbf{q}) - \tilde{n}_n^{(\text{in})}(\mathbf{q}),$$

$$F = \langle \bar{R}_{n+1} | \bar{R}_{n+1} \rangle - \lambda \left(1 - \sum_m^n a_m \right),$$

$$\langle R_m | R_{m'} \rangle \equiv \sum_{\mathbf{q}} \frac{R_m^*(\mathbf{q}) R_{m'}(\mathbf{q})}{w(\mathbf{q})},$$

$$= \sum_{m,m'} \alpha_m \alpha_{m'} \langle R_m | R_{m'} \rangle - \lambda \left(1 - \sum_m^n a_m \right).$$

Kerker factor

$$w(\mathbf{q}) = \frac{|\mathbf{q}|^2}{|\mathbf{q}|^2 + q_0^2},$$

Minimization of F leads to

Long wave length components corresponding to small $|\mathbf{q}|$ are taken into account.

$$\frac{\partial F}{\partial \alpha_k} = 0 \quad \left(\begin{array}{ccccc} \langle R_{n-(p-1)} | R_{n-(p-1)} \rangle & \cdots & \cdots & 1 \\ \cdots & \cdots & \cdots & 1 \\ \cdots & \cdots & \langle R_n | R_n \rangle & \cdots \\ 1 & 1 & \cdots & 0 \end{array} \right) \left(\begin{array}{c} \alpha_{n-(p-1)} \\ \alpha_{n-(p-1)+1} \\ \vdots \\ \frac{1}{2}\lambda \end{array} \right) = \left(\begin{array}{c} 0 \\ 0 \\ \vdots \\ 1 \end{array} \right).$$

Optimum input density might be given by

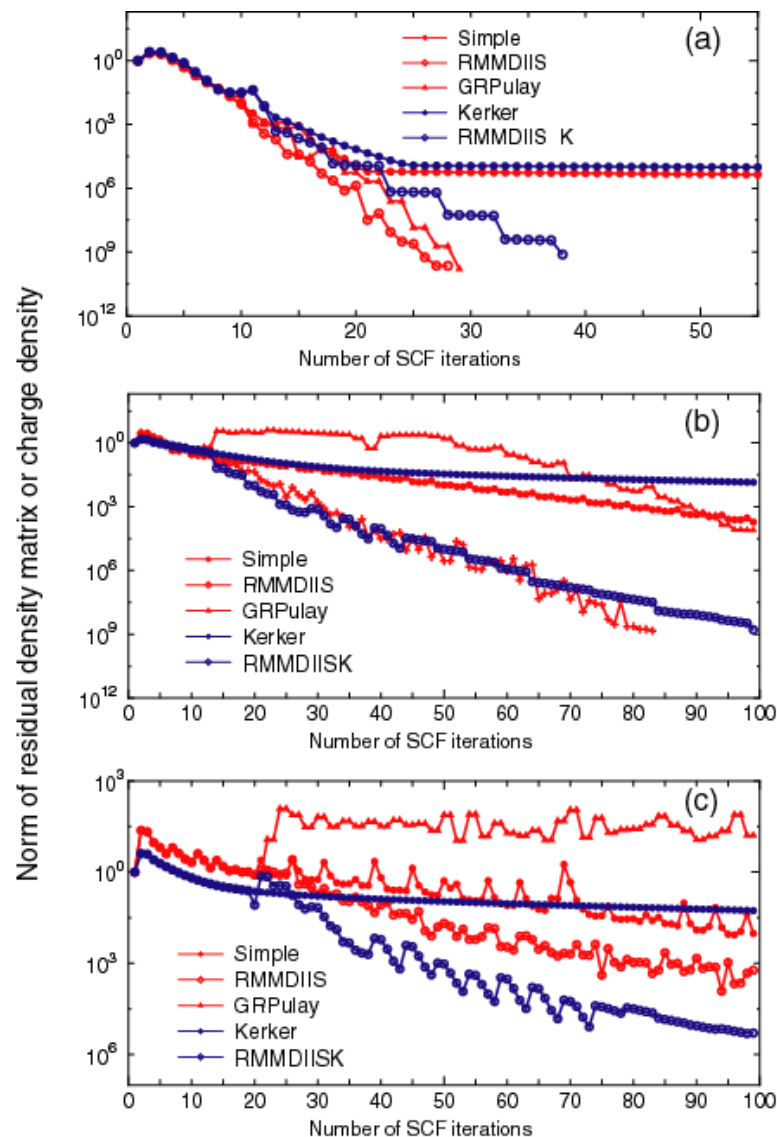
$$\rho_{n+1}^{(\text{in})} = \sum_{m=n-(p-1)}^n \alpha_m \rho_m^{(\text{in})} + \beta \sum_{m=n-(p-1)}^n \alpha_m R_m$$

Comparison of various mixing methods

Sialic acid

Pt₁₃ cluster

Pt₆₃ cluster



RMM-DIIS shows better performance.

Reproducibility in DFT calcs

RESEARCH ARTICLE

Science 351, aad3000 (2016)

DFT METHODS

Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere,^{1*} Gustav Bihlmayer,² Torbjörn Björkman,^{3,4} Peter Blaha,⁵ Stefan Blügel,² Volker Blum,⁶ Damien Caliste,^{7,8} Ivano E. Castelli,⁹ Stewart J. Clark,¹⁰ Andrea Dal Corso,¹¹ Stefano de Gironcoli,¹¹ Thierry Deutsch,^{7,8} John Kay Dewhurst,¹² Igor Di Marco,¹³ Claudia Draxl,^{14,15} Marcin Dułak,¹⁶ Olle Eriksson,¹³ José A. Flores-Livas,¹² Kevin F. Garrity,¹⁷ Luigi Genovese,^{7,8} Paolo Giannozzi,¹⁸ Matteo Giantomassi,¹⁹ Stefan Goedecker,²⁰ Xavier Gonze,¹⁹ Oscar Grånäs,^{13,21} E. K. U. Gross,¹² Andris Gulans,^{14,15} François Gygi,²² D. R. Hamann,^{23,24} Phil J. Hasnip,²⁵ N. A. W. Holzwarth,²⁶ Diana Iuşan,¹³ Dominik B. Jochym,²⁷ François Jollet,²⁸ Daniel Jones,²⁹ Georg Kresse,³⁰ Klaus Koepernik,^{31,32} Emine Küçükbenli,^{9,11} Yaroslav O. Kvashnin,¹³ Inka L. M. Locht,^{13,33} Sven Lubeck,¹⁴ Martijn Marsman,³⁰ Nicola Marzari,⁹ Ulrike Nitzsche,³¹ Lars Nordström,¹³ Taisuke Ozaki,³⁴ Lorenzo Paulatto,³⁵ Chris J. Pickard,³⁶ Ward Poelmans,^{1,37} Matt I. J. Probert,²⁵ Keith Refson,^{38,39} Manuel Richter,^{31,32} Gian-Marco Rignanese,¹⁹ Santanu Saha,²⁰ Matthias Scheffler,^{15,40} Martin Schlöf,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*}

15 codes

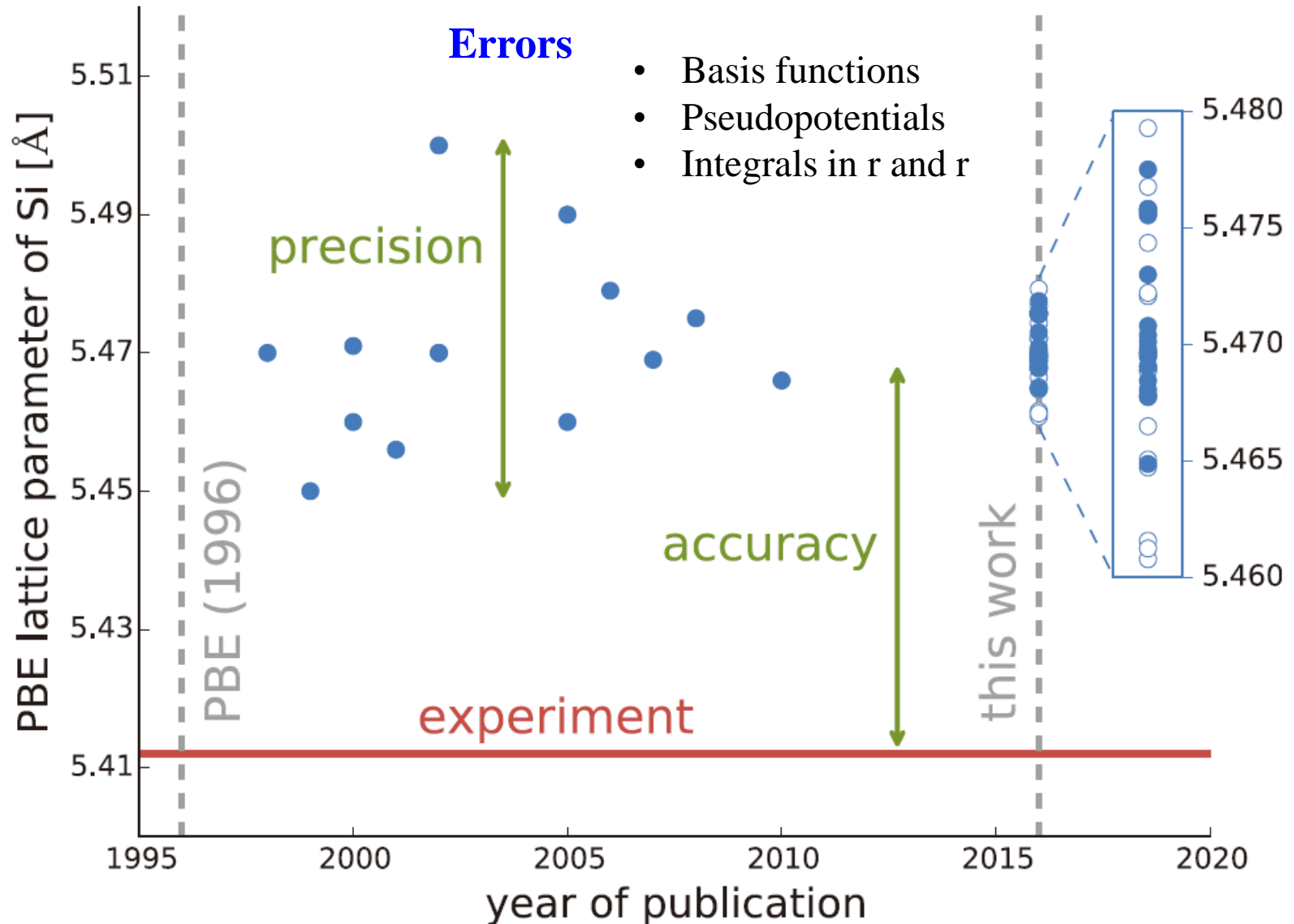
69 researchers

71 elemental bulks

GGA-PBE

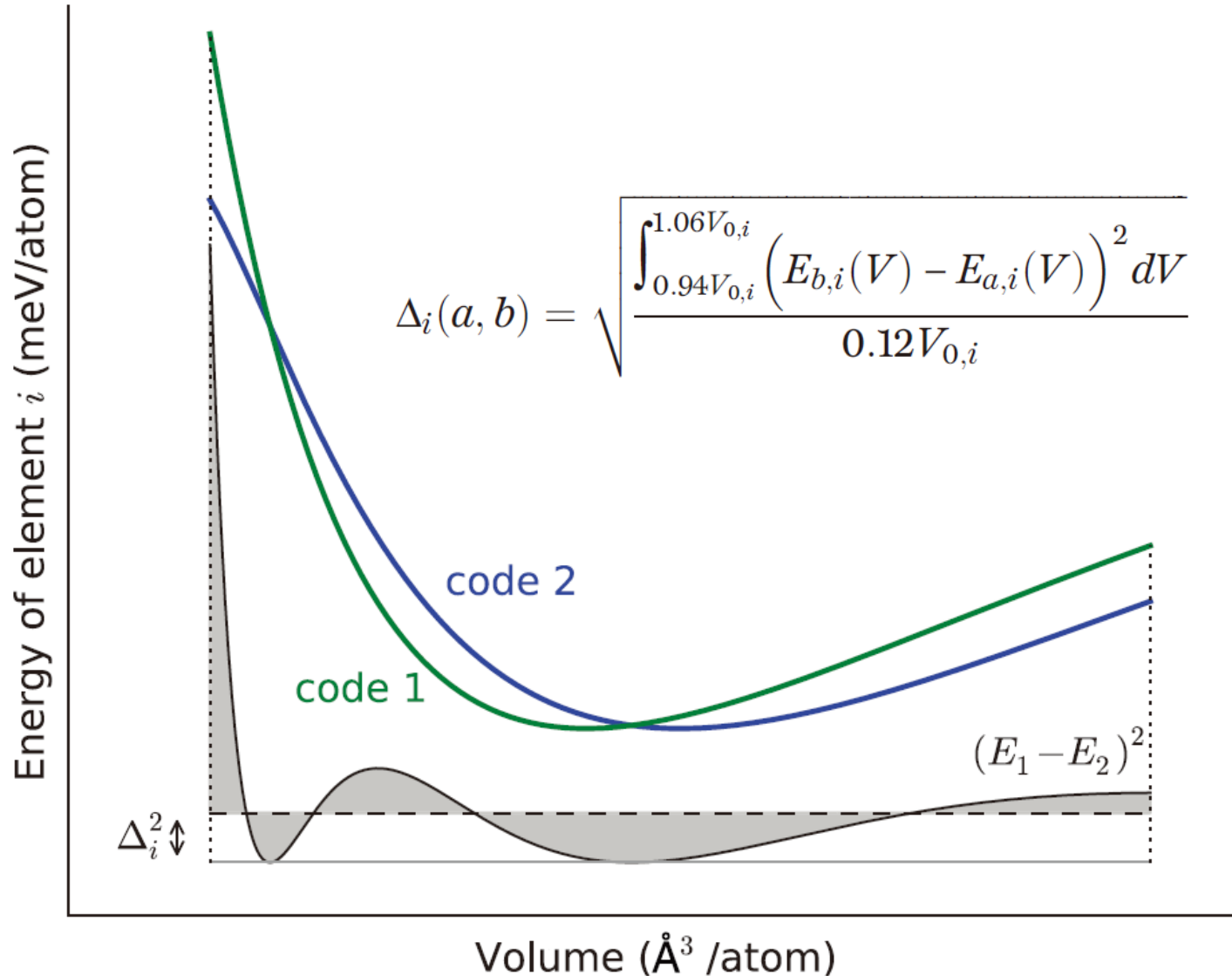
Scalar relativistic

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
Li	Be	$\Delta(\text{exp}) = 23.5 \text{ meV/atom}$										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
	PS11b100/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.

Outlook

- A localized basis method, implemented in OpenMX, was discussed with the following focuses:
 - Total energy
 - Pseudopotentials
 - Basis functions
 - Self-consistency
- The careful evaluation of the total energy and optimization of PPs and PAOs guarantee accurate and fast DFT calculations in a balanced way.