Atomic-orbital Based Ab-initio simulations

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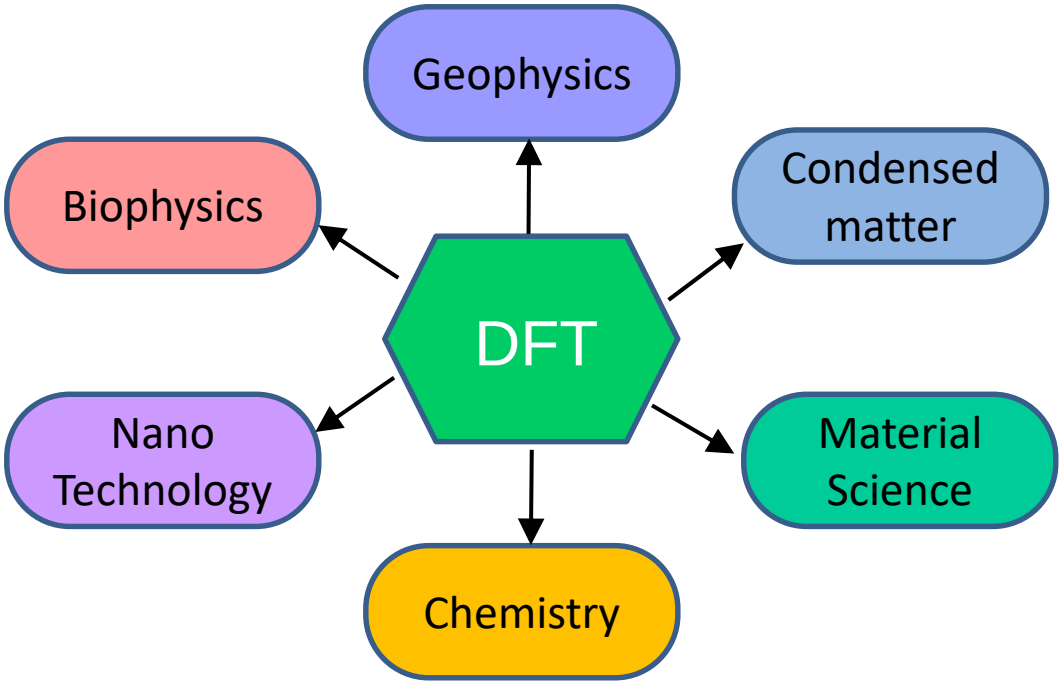
The **Nobel Prize** in **Chemistry 1998** was awarded to W. Kohn "for his development of the density-functional theory".

1923/3/9-2016/4/19

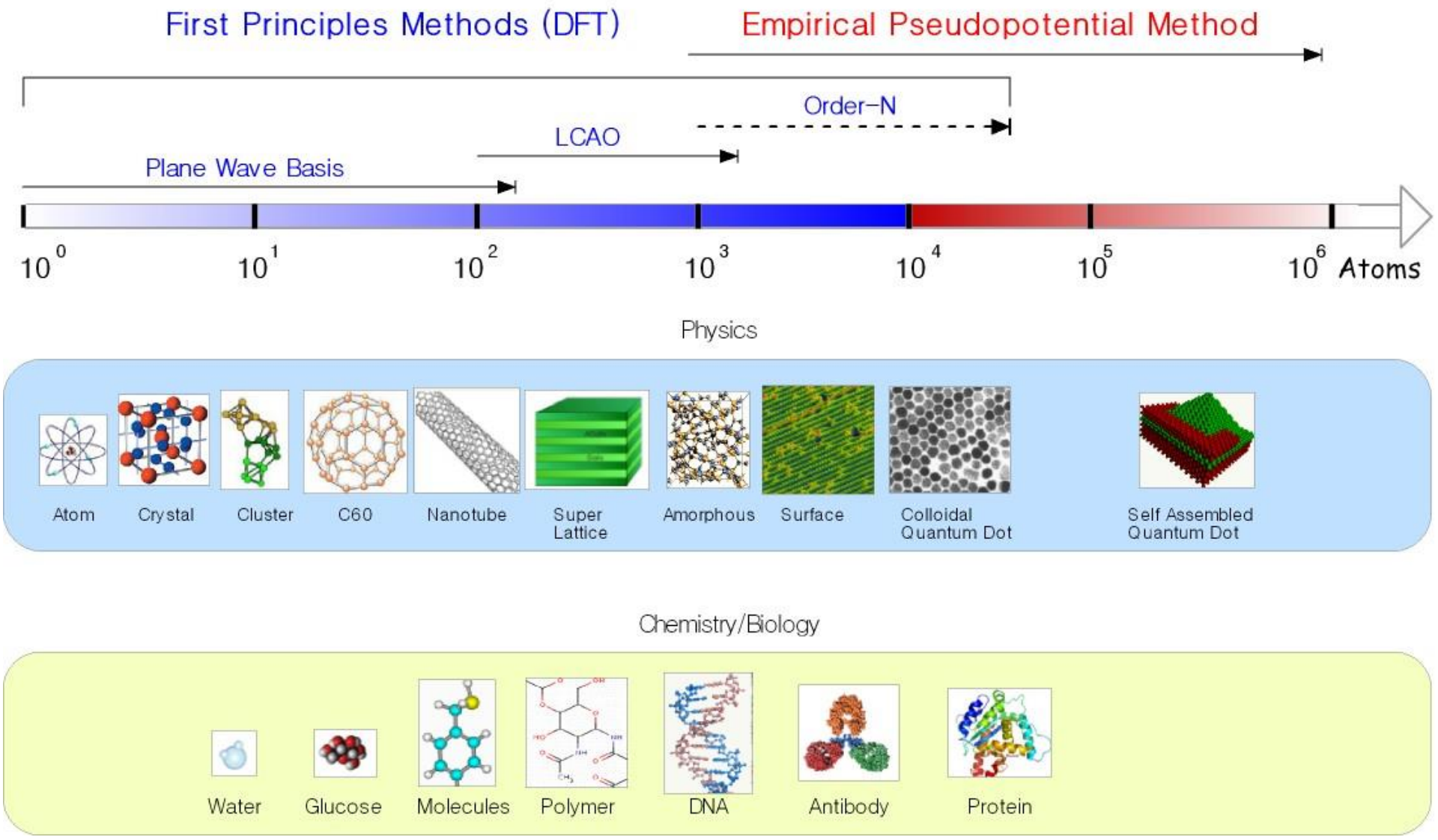
◆Applications：



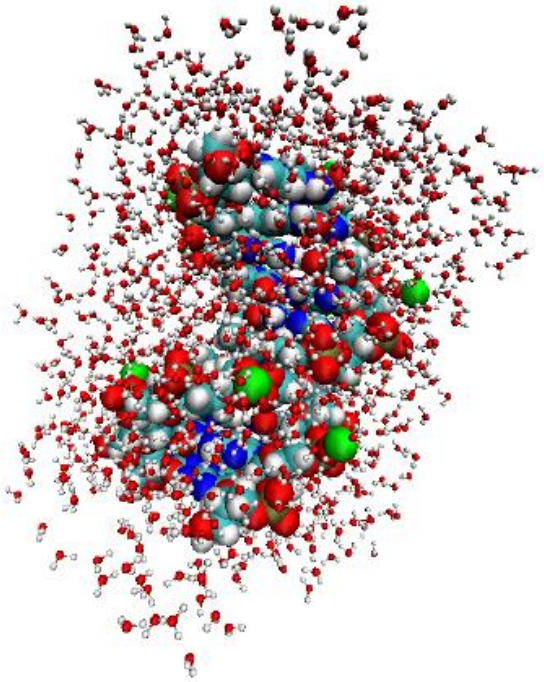
◆New developments：

New functionals：more accurate
Numerical methods：larger systems

The development of first-principles methods

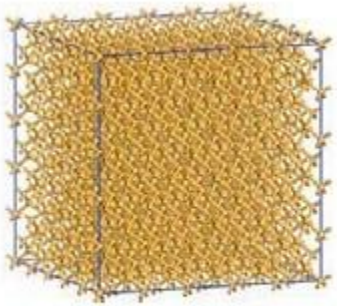


Application of DFT for thousands of atoms

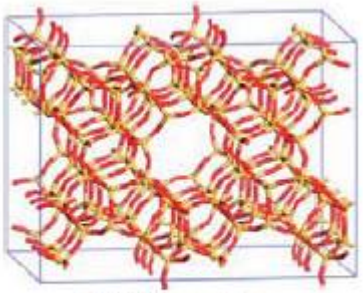


DNA containing 3439 atoms

J. Phys. : Condens. Matter **20** (2008) 294201 (CONQUEST)

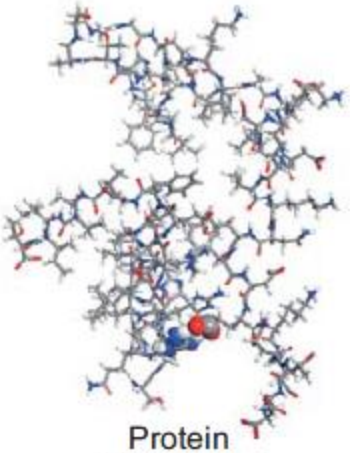


Crystalline silicon
(1000 atoms)

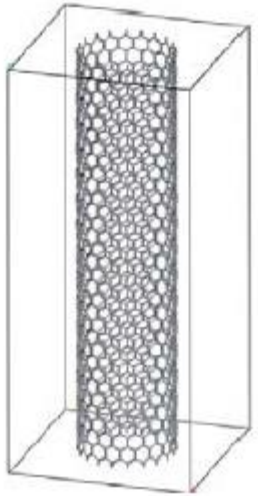


ZSM5 zeolite
(576 atoms)

Phys. stat. sol. (b) **243,** No.5 (2006) 977 (ONETEP)



Protein
(988 atoms)



(20, 0) Nanotube
(1280 atoms)

Kohn-Sham equation

$$\left[-\frac{\nabla^2}{2m} + V_{Hxc}[n](r) + V_{ext}(r) \right] \varphi_i(r) = \varepsilon_i \, \varphi_i(r)$$

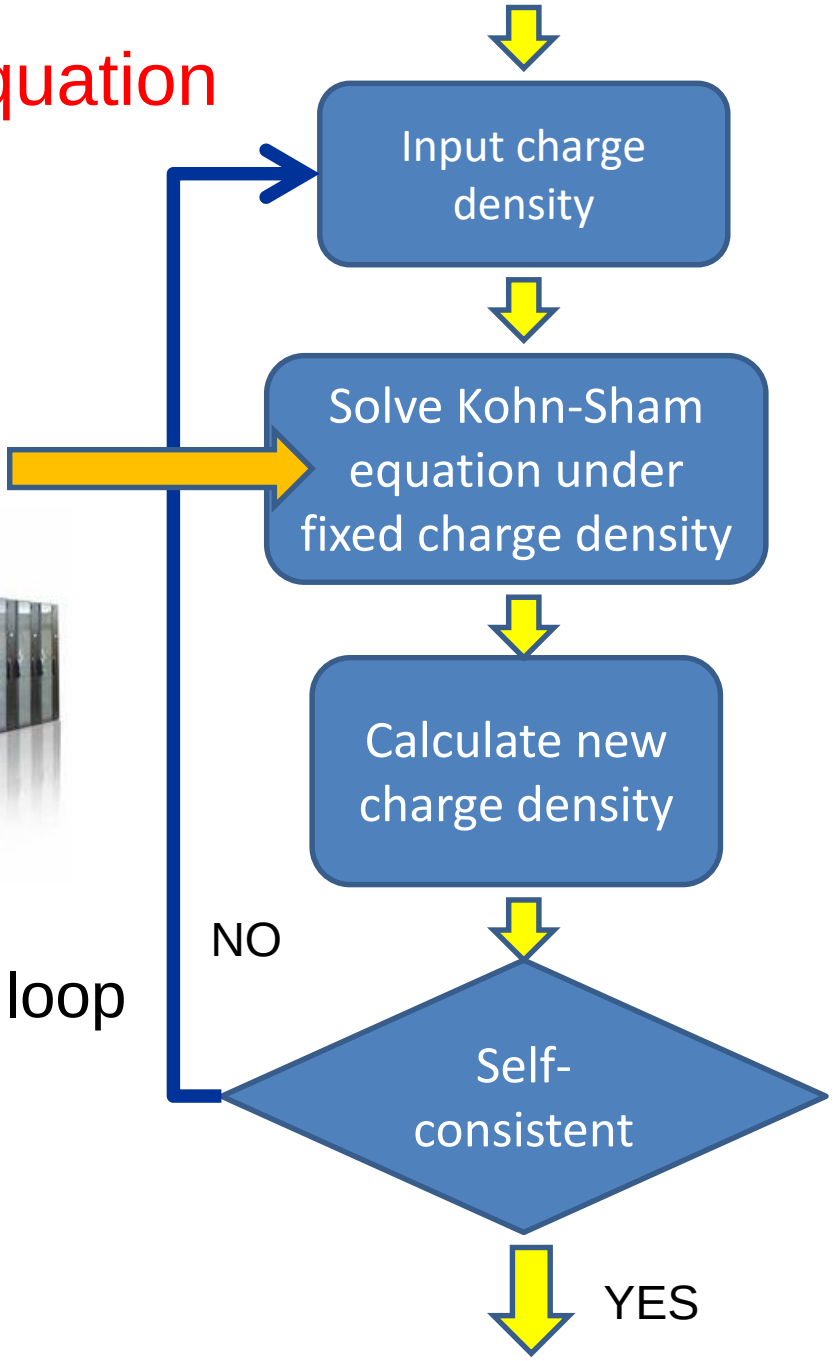
$$V_{Hxc}[n] = \frac{\delta E_{Hxc}[n]}{\delta n} \qquad n(r) = \sum_i^{\text{occ}} \left| \varphi_i(r) \right|^2$$

KS equation maps the many-particle problem into a single-particle problem. The mapping is exact, if the energy functional is exact!

Solving Kohn-Sham equation

Most time consuming step

Self-consistent loop



Solve Kohn-Sham equation

By choosing proper basis set, one can turn the Kohn-Sham equation to a matrix eigenvalue problem

$$|\psi_i\rangle = \sum_{q'} c_{i,q'} |q'\rangle$$

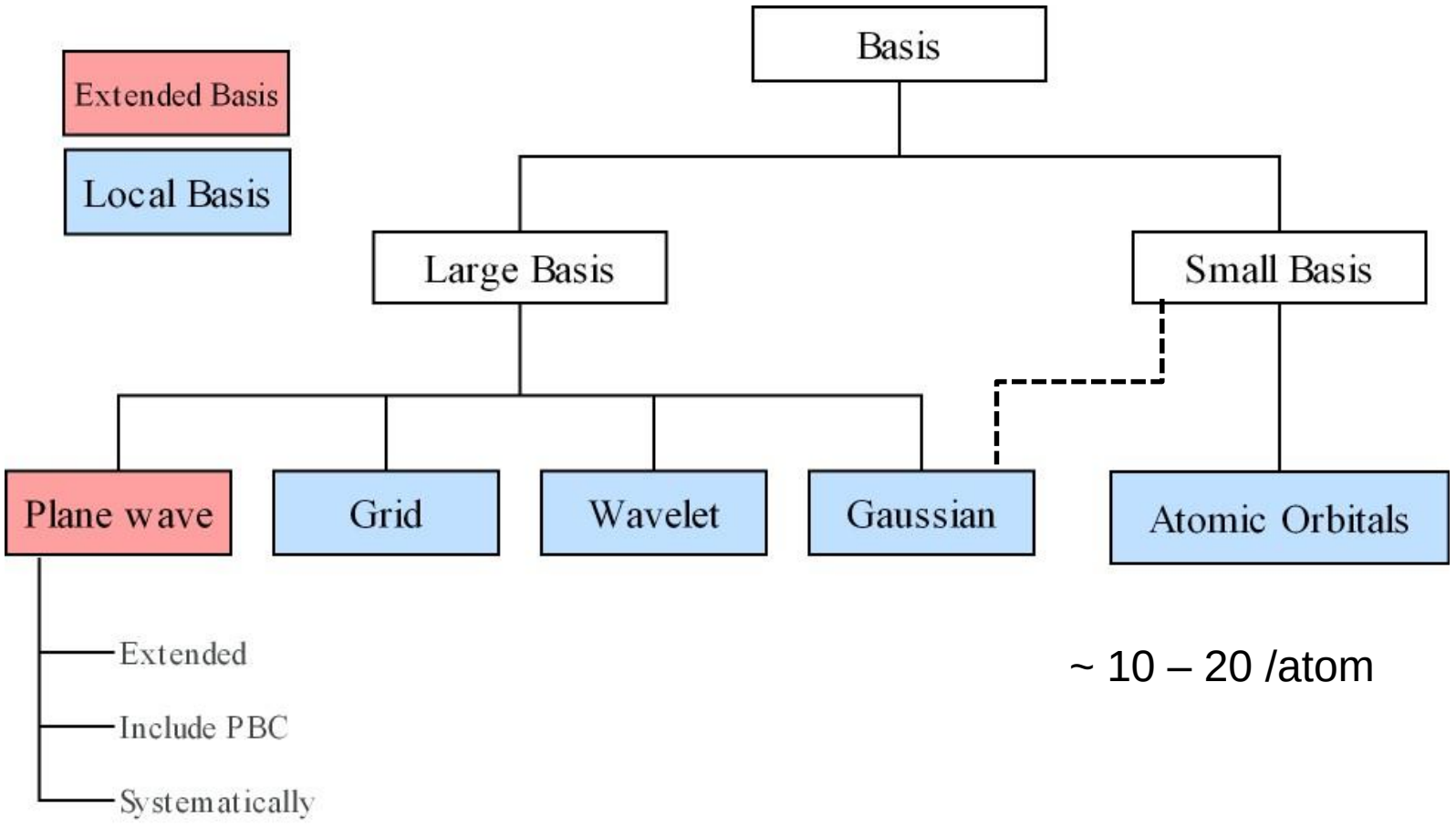
$$\sum_{q'} \langle q|H|q'\rangle c_{i,q'} = \varepsilon_i \sum_{q'} c_{i,q'} \langle q|q'\rangle$$

$$\rightarrow \quad \sum_{q'} H(q,q')\, c_{i,q'} = \varepsilon_i \sum_{q'} S(q,q') c_{i,q'}$$

One of the central problems for designing efficient electronic structure algorithm is to find proper basis sets

- All electron: APW, MTO
- Pseudopotential: Plane wave, atomic orbital, etc.

Popular basis sets



~ 10 – 20 /atom

~ 500 – 1000 /atom

Plane wave basis (PWB)

- ☺ Independent of atom positions, easy to implement.
- ☺ Forces can be easily calculated.
- ☺ Can be systematically improved by a single parameter (Ecut)
- ☺ Efficient for <100 atoms.
- ☹ Inefficient for large systems: O(N^3).

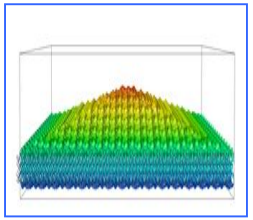
VASP b-initio ackage ienna imulation

PWscf

abinit

Some DFT packages for thousands of atoms

CONQUEST
(England and Japan)



Basis : Numerical orbtials
/ finite element basis

ONETEP
(England)

Basis : real space grid/
Wannier functions

SIESTA
(Spain)

Basis : Numerical orbitals

OpenMX
(Japan)

Basis : Numerical orbitals

FHI-aims
(Germany, FHI)

Basis : Numerical orbitals
All electron code

Bloch wave function in plane wave bases

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{G})$$

Bloch wave function in numerical atomic orbital bases (LCAO)

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

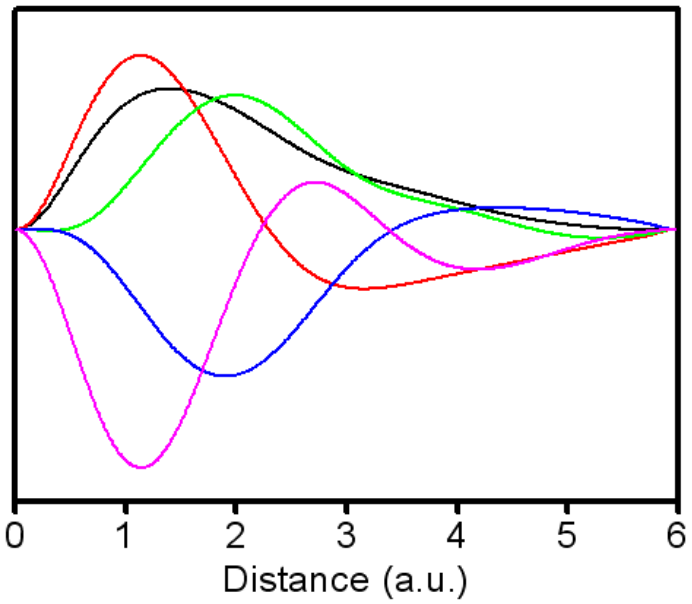
NAO

Atomic orbitals

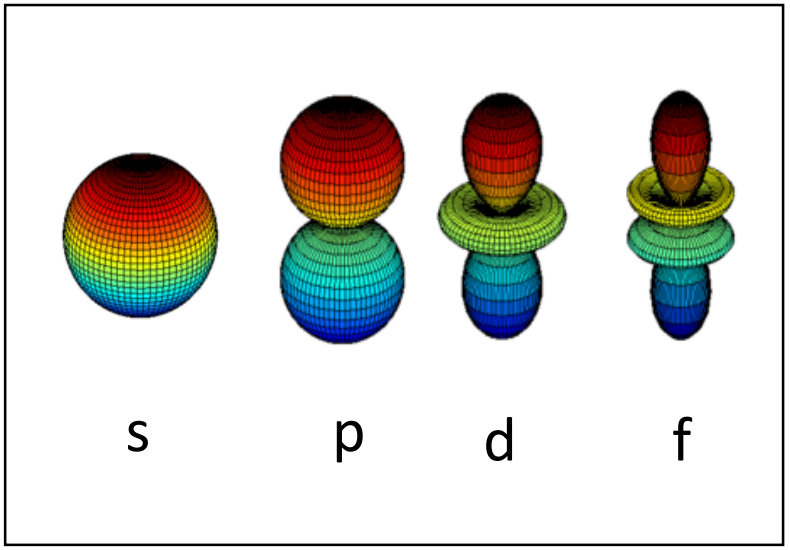
$$\phi_{I,l,m,n}(\vec{r}) = R_{I,l,n}(r)Y_{l,m}(\hat{r}_I)$$

Radial wave functions

(size, range, shape)



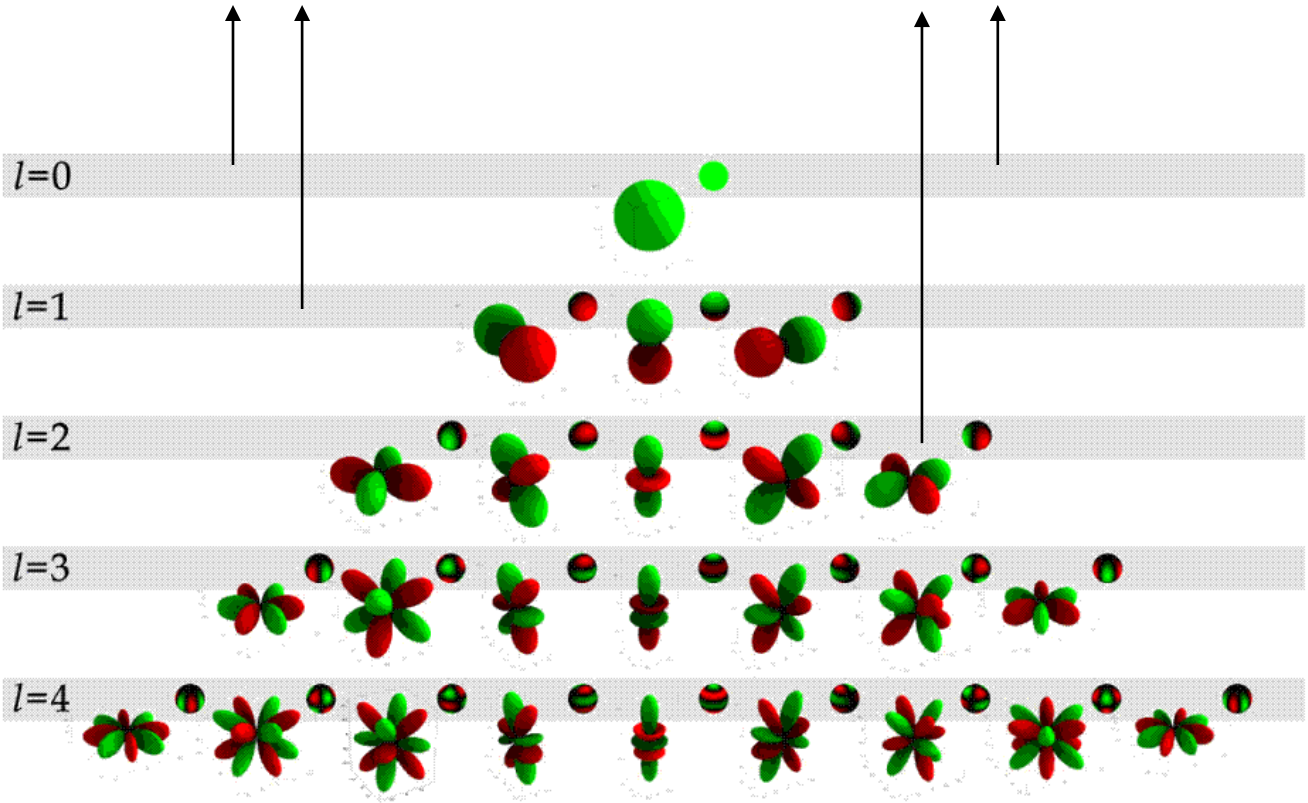
Spherical harmonics



Adapt to any symmetry!

Examples of atomic orbitals

	Carbon (4 orbitals)	Manganese (6 orbitals)
core	$1s^2$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$
valence	$2s^2 2p^4$	$3d^5 4s^2$



How to improve the atomic basis sets

Low Accuracy

High Accuracy

(need more computational resource)

Minimal basis set

Multiple-zeta orbitals

+

Polar orbitals

Advantages

- Small basis sets.
- Local basis, suitable for O(N) algorisms.

Two problems

- Accuracy
- Transferability

Systematically improvable?

Atomic basis sets

◆**Multi-zeta orbitals**: Different radial wave functions for the same angular momentum

◆**Polar orbitals:** Orbitals with higher angular momentum than valence orbitals.

■ **Systematically improvement**: ‘SZ’, ‘DZ’, ‘DZP’ , ‘TZDP’…

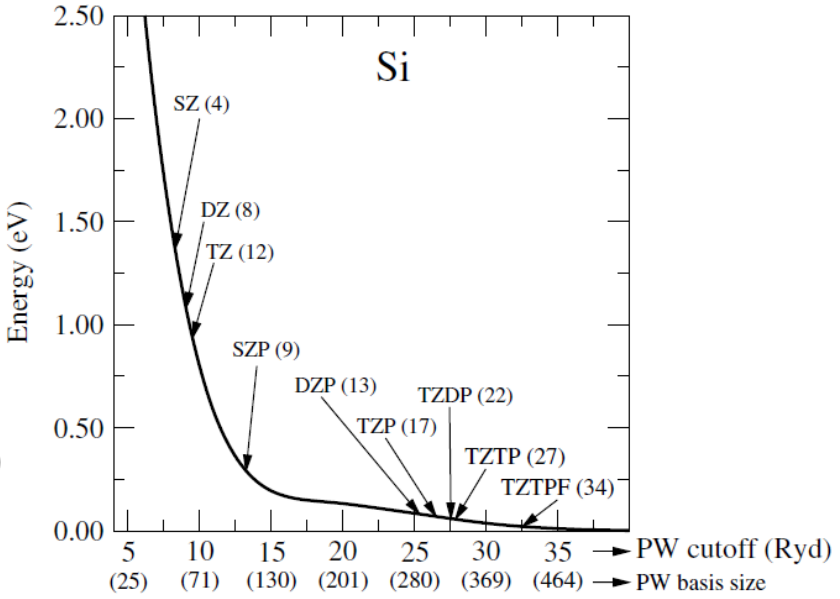
SZ: Single-zeta (minimal basis set sp)

DZ: Double-zeta (2s2p)

DZP: Double-zeta + Polar orbital (2s2p1d)

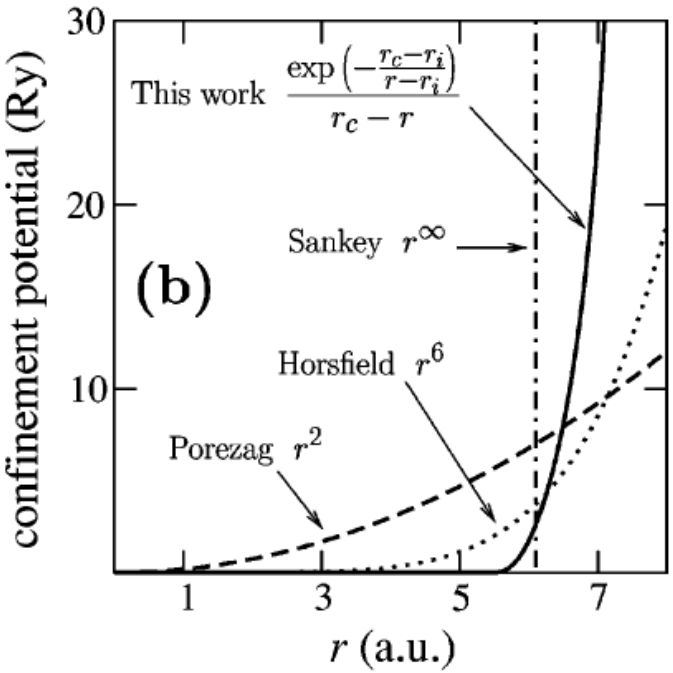
TZDP: Triple-zeta + double Polar orbital (3s3p2d)

Taken Si as an example

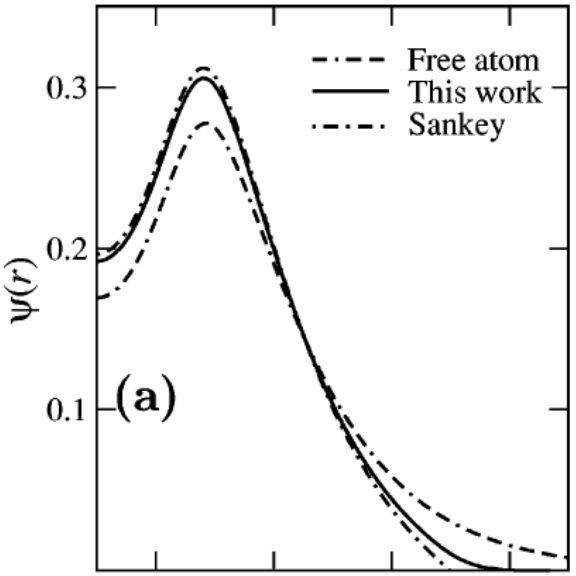


How to construct atomic orbitals

$$\left[-\frac{\nabla^2}{2}+V_{atom}(r)+V_{confine}(r)\right]\phi_{lm}(r)=\varepsilon_n\phi_{lm}(r)$$



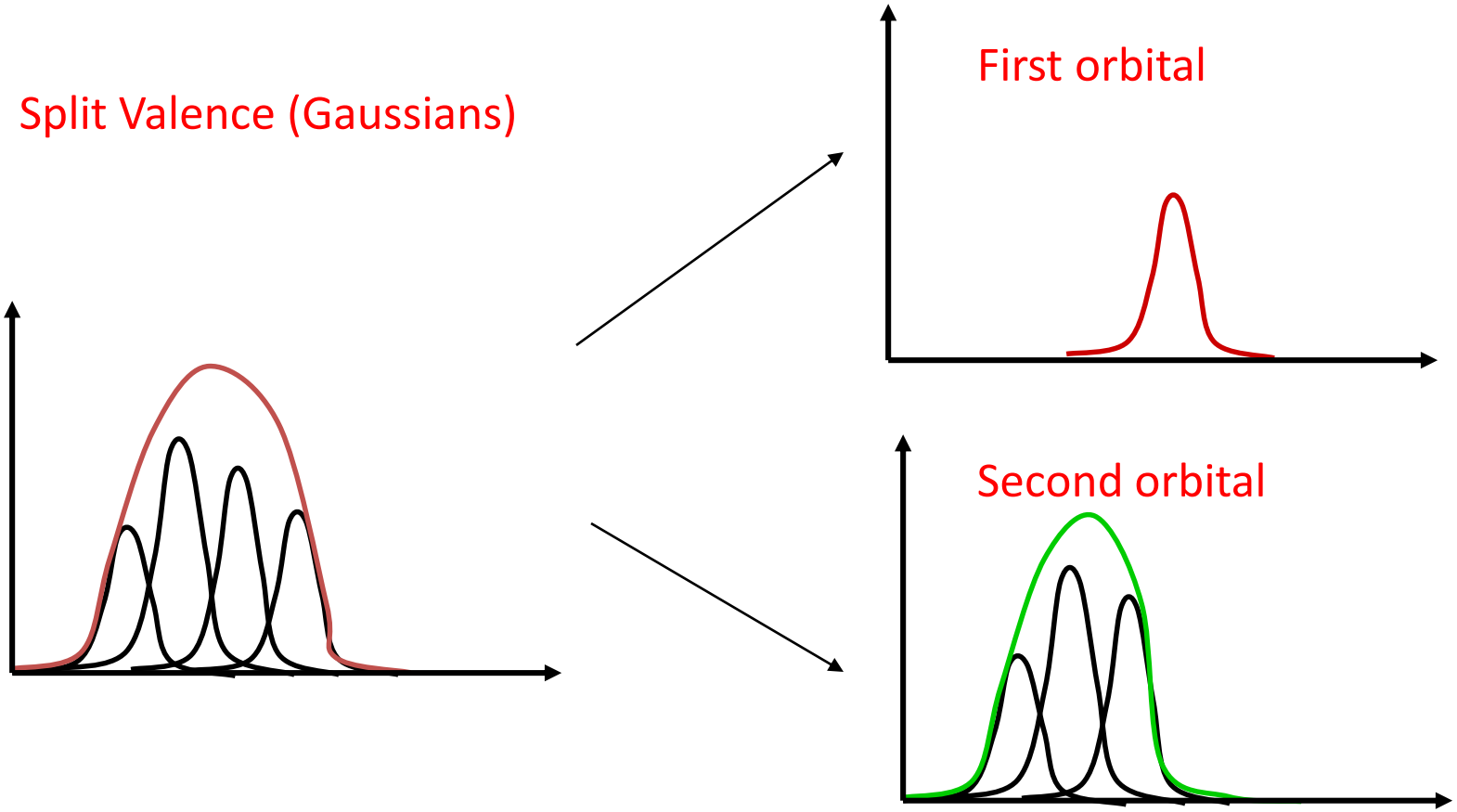
Confinement potential



The shape of orbitals

J. Junquera et al, Phys Rev B **64**, 235111 (2001)

How to construct multi-zeta orbitals



Pablo Ordejon, Summer schoold of SIESTA, 2007

How to construct polarized orbitals

Method 2: Apply electric field

$$\left[-\frac{\nabla^2}{2}+V_{atom}(r)+V_{confine}(r)+E\cdot r\right]\psi_n=\varepsilon_n\psi_n$$

Selection rule

$$\left[\frac{1}{2r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r+\frac{(l+1)(l+2)}{2r^2}+V_r(l)-E_l\right]\phi_{l+1}=-\epsilon r\phi_l(r)c_{l+1}$$

J. Soler et al, J. phys: Condens. Matter. **14**, 2745 (2002)

How to construct polar orbitals

Compare method 1 and method 2

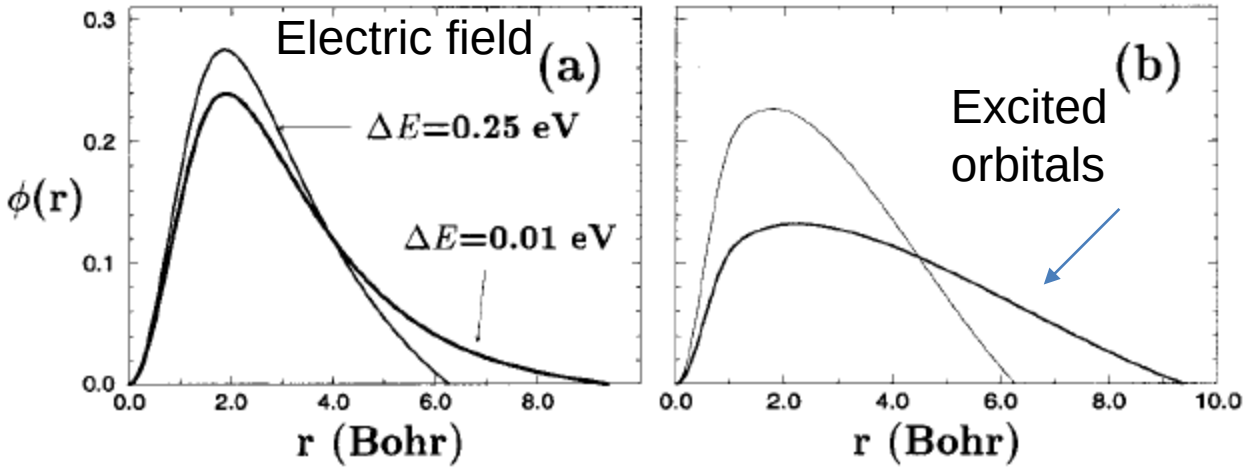


Fig. 3. d polarization orbitals for silicon for two different confinement conditions. a) Obtained with the electric-field polarization method and b) the confined d PAOs

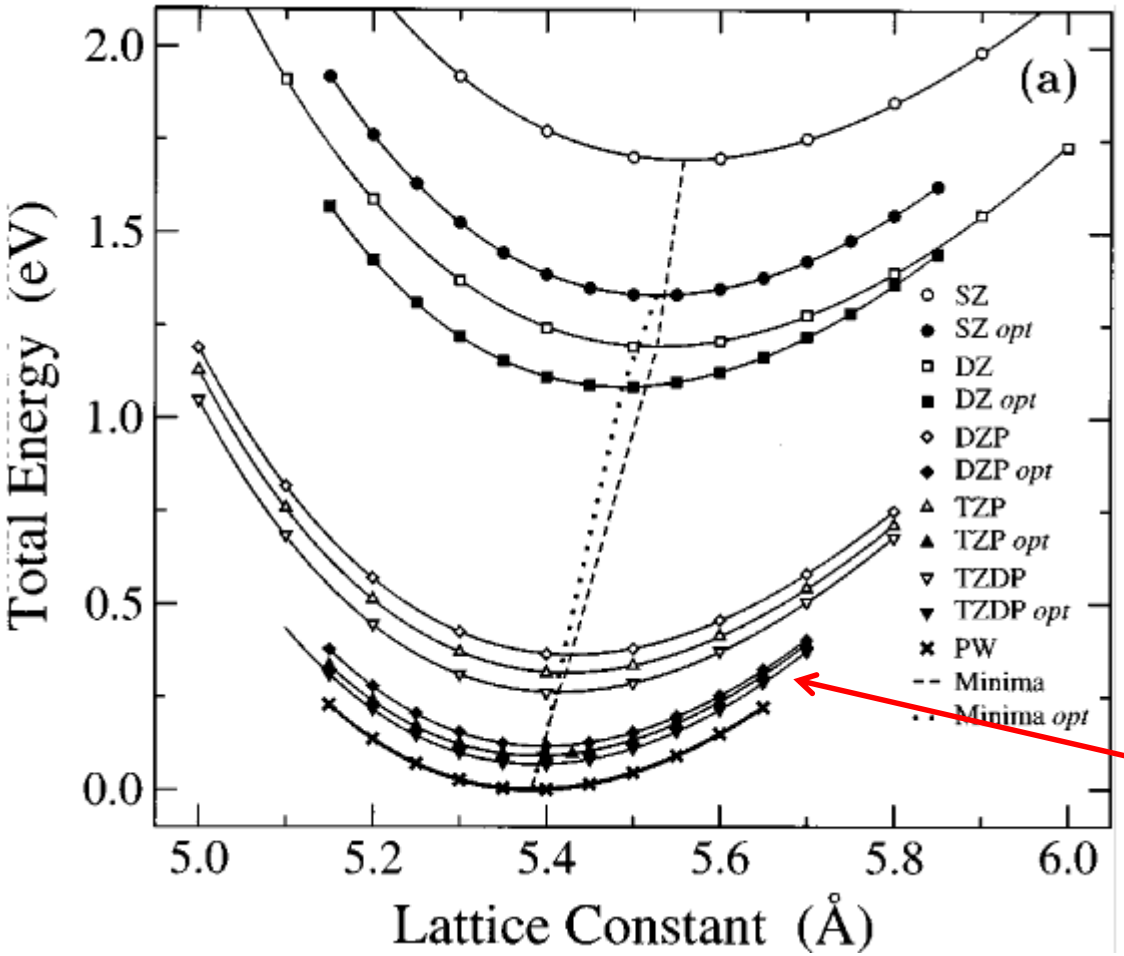
Scheme (2)

Scheme (1)

E. Artacho et al, Phys. Stat. Sol. (b) **215**, 809 (1999)

Test atomic basis on bulk Si

Bulk Silicon



Optimized

J. Junquera et al, Phys Rev B **64**, 235111 (2001)

Problems of previous orbital generation methods

1. Complicated especially for multi-zeta and polar orbtials.

2. The orbitals are not fully optimized.

Our Method: spillage minimization

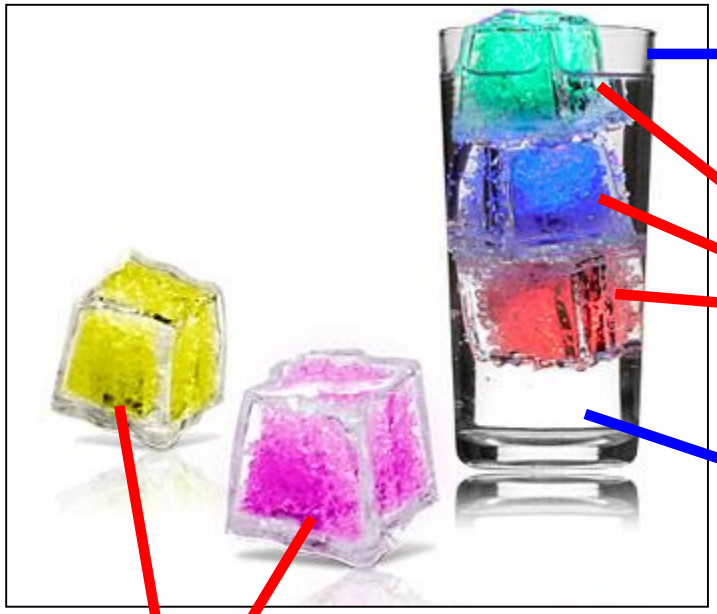
What is "Spillage":

$$\mathcal{S} = \frac{1}{N_n}\sum_{n=1}^{N_n}\langle\Psi_n|1-\hat{P}|\Psi_n\rangle$$

→ Reference states

$$\hat{P} = \sum_{\mu\nu}|\phi_\mu\rangle S^{-1}_{\mu\nu}\langle\phi_\nu|$$

Local orbital space



Cup: Hilbert Space spanned by reference states (plane wave).

Hilbert Space spanned by Local orbitals

Hilbert space left： spillage

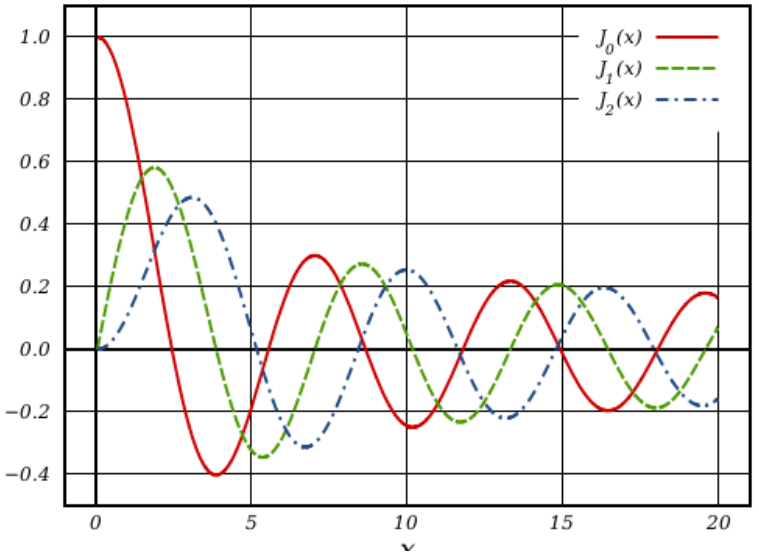
Ice Block： atomic orbitals

D. S. Portal, et al. Solid State Communications **95**, 685 (1995)

Radial functions

Spherical Bessel functions:

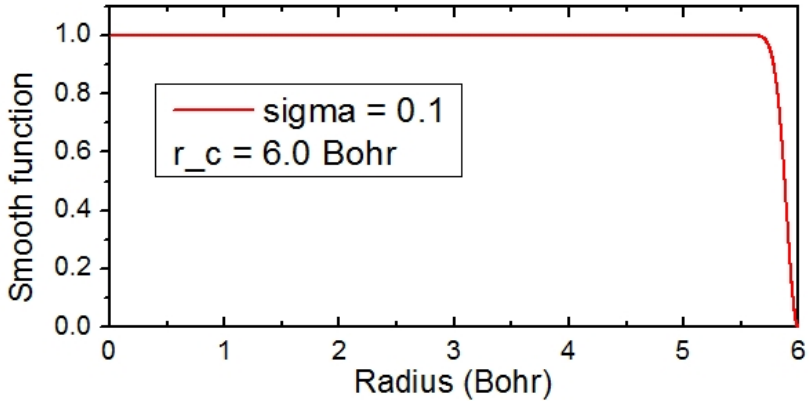
$$f_{\mu,l}(\mathbf{r}) = \begin{cases} \sum_q c_{\mu q} j_l(qr), & r < r_c \\ 0 & r \geq r_c \end{cases}$$



Very flexible!

To ensure continuity, multiply f by a smooth function:

$$g(r) = 1 - \exp[-\frac{(r - r_{\text{cut}})^2}{2\sigma^2}]$$

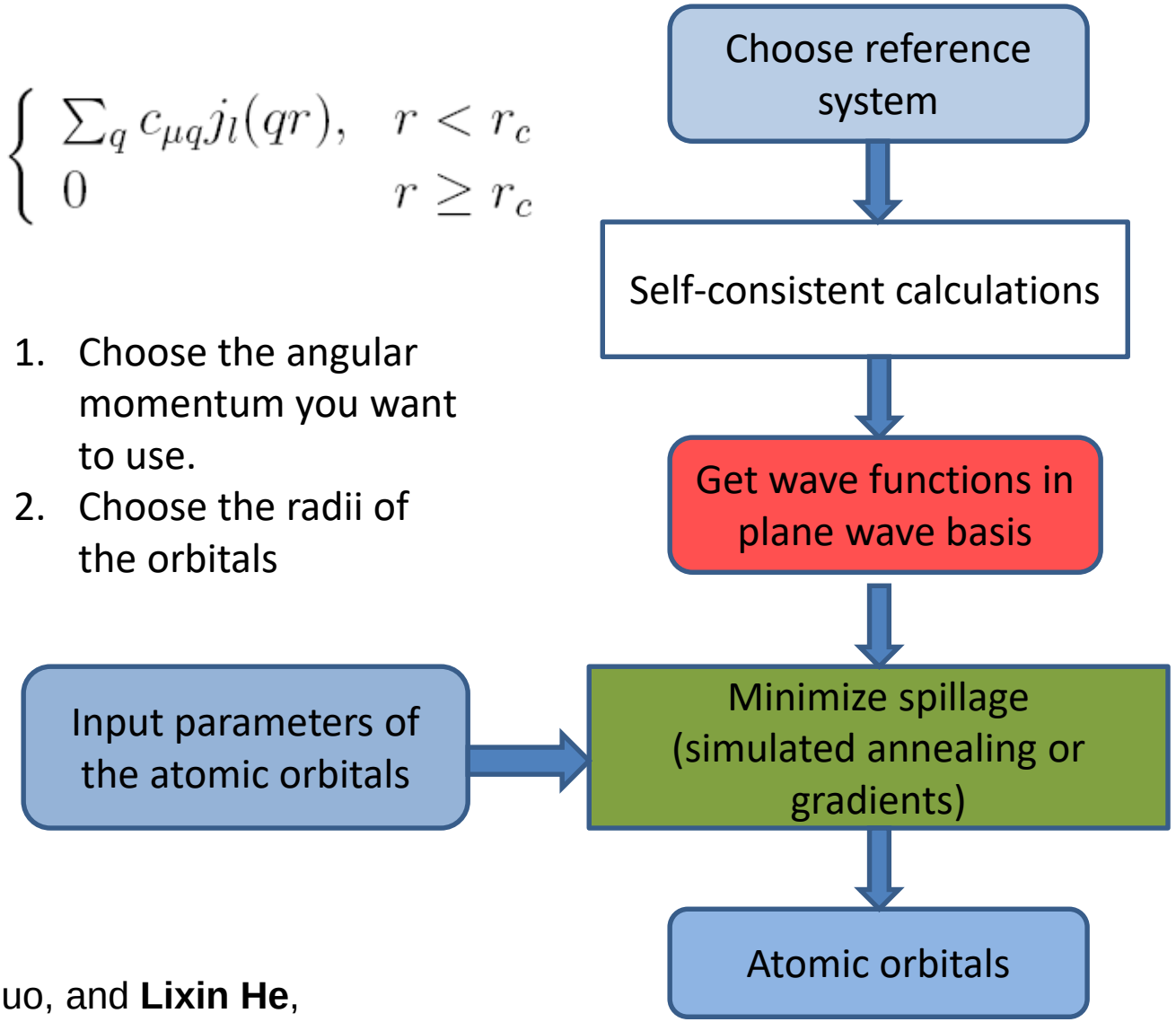


Mohan Chen, G-C Guo, and **Lixin He**, *J. Phys.: Cond. Matt.* **22** 445501 (2010)

Steps to get the orbitals

$$f_{\mu,l}(\mathbf{r}) = \begin{cases} \sum_q c_{\mu q} j_l(qr), & r < r_c \\ 0 & r \geq r_c \end{cases}$$

1. Choose the angular momentum you want to use.
2. Choose the radii of the orbitals

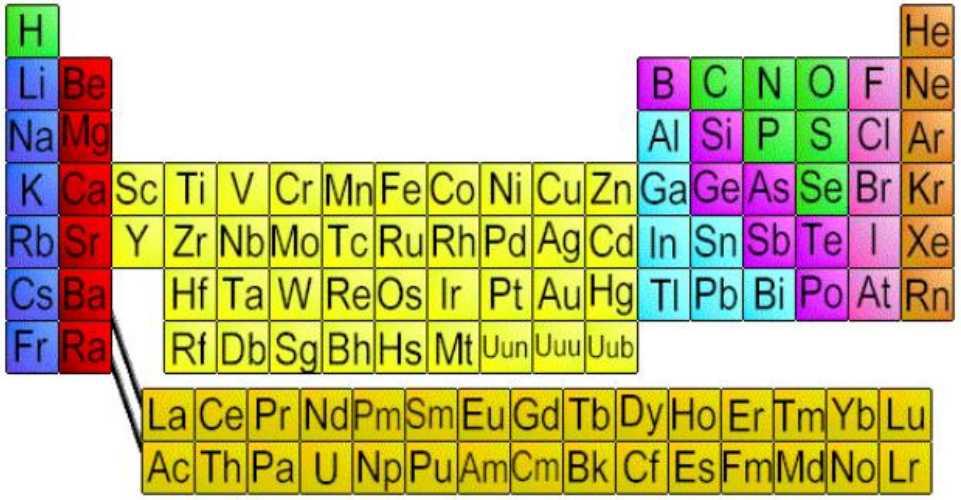


Mohan Chen, G-C Guo, and **Lixin He**,
J. Phys.: Cond. Matt. **22** 445501 (2010)

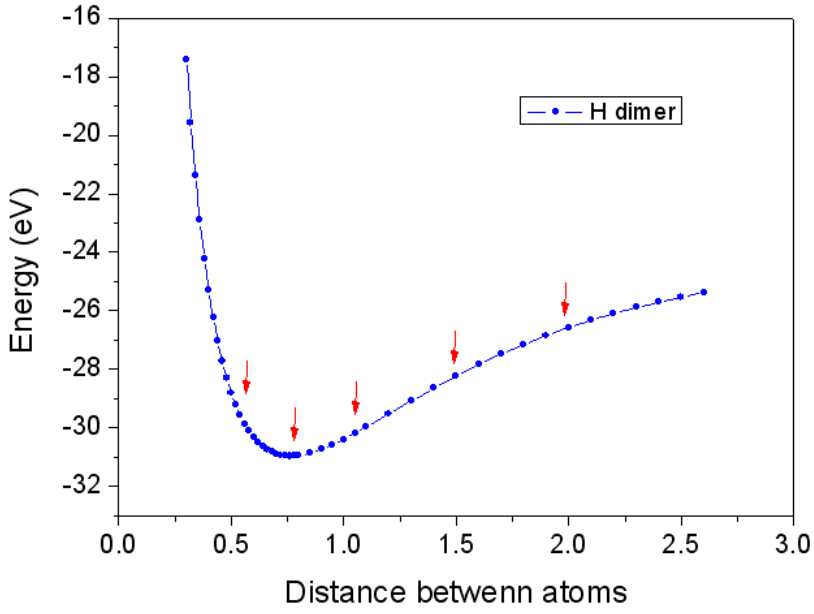
Reference system: dimers

Molecule made of two identical atoms: “dimer”

No bias!



- Choose a set of dimers with different bond lengths.
- Calculate the energies and wave functions
- 4~5 dimers are enough to get good orbitals

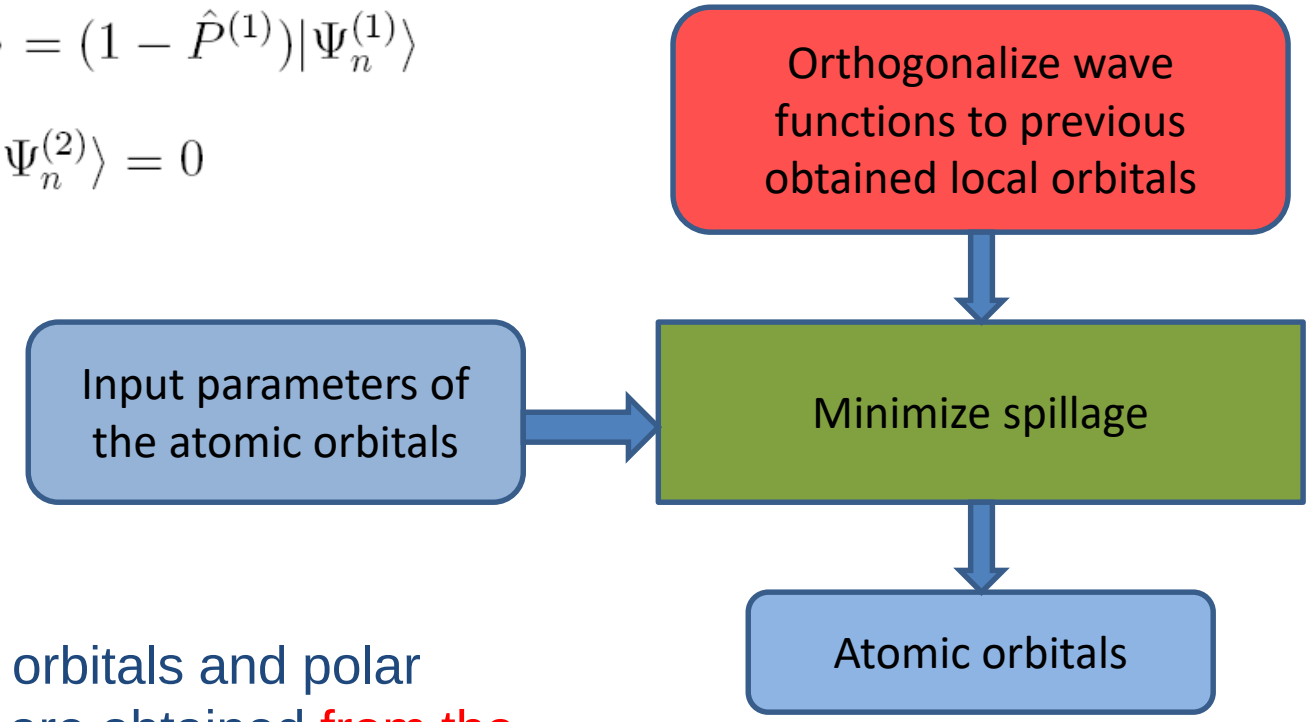


Systematically generate atomic basis

$$\hat{P}^{(1)} = \sum_{\mu\nu} |\phi_\mu^{(1)}\rangle S_{\mu\nu}^{-1} \langle\phi_\nu^{(1)}|$$

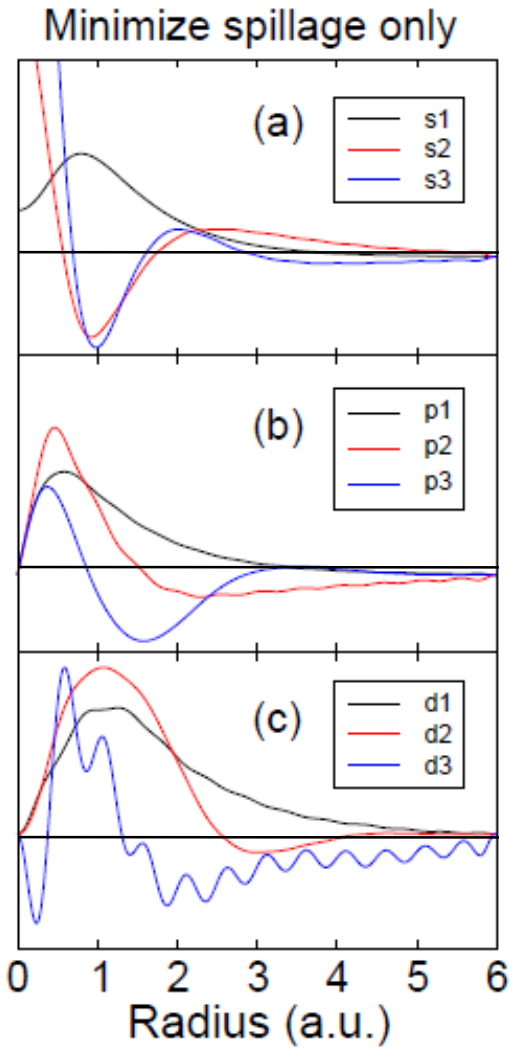
$$|\Psi_n^{(2)}\rangle = (1 - \hat{P}^{(1)})|\Psi_n^{(1)}\rangle$$

$$\hat{P}^{(1)}|\Psi_n^{(2)}\rangle = 0$$



All zeta orbitals and polar orbitals are obtained from the same procedure!

The radial functions of Carbon (6.0 Bohr)



SCF with:

- Carbon dimers of 5 bond lengths.
- LDA
- Energy cutoff = 100 Ry

Radial functions have oscillation!

Unphysical + worsen the transferability of the basis

Optimize the orbital shape

- Minimize “kinetic energy” of the orbitals

$$\min\left[\mathrm{T}_{\mu}(c_{\mu q})\right] = \min\left[\sum_{q} c_{\mu q}^{2} q^{2} / 2 + \kappa\right]$$

$$\kappa = \begin{cases} 0, & \mathcal{S}/\mathcal{S}_0 - 1 < \Delta \\ \infty, & \mathcal{S}/\mathcal{S}_0 - 1 > \Delta \end{cases}$$

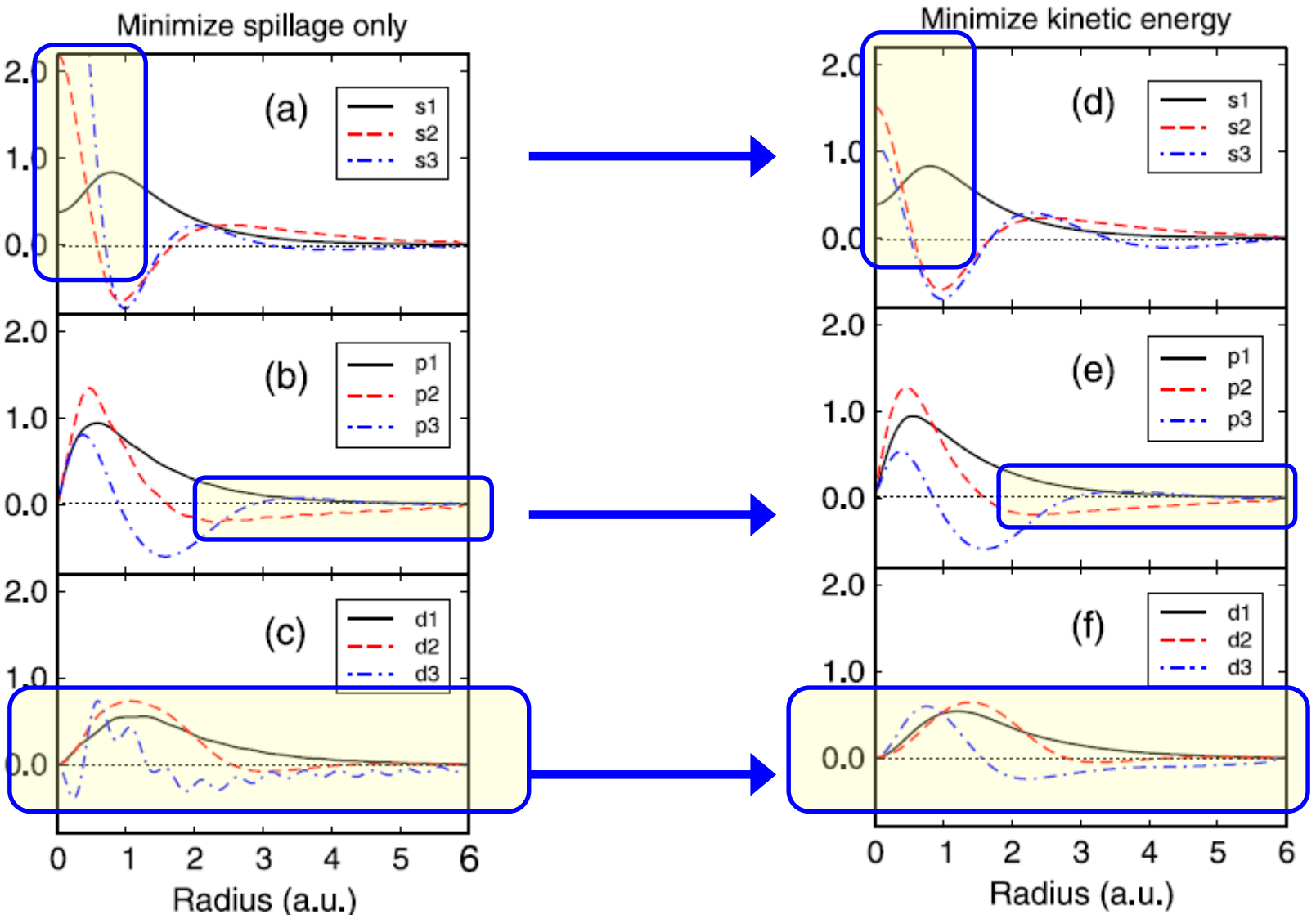
(0.002~0.005 is enough)

S: Current Spillage

S0: Spillage before minimize kinetic energy.

Mohan Chen, G-C Guo, and **Lixin He**, *J. Phys.: Cond. Matt.* **22** 445501 (2010)

Optimized radial functions for Carbon



Spillage vs. Total energy

Increase atom radii
(4 a.u. -> 12 a.u.)

↓

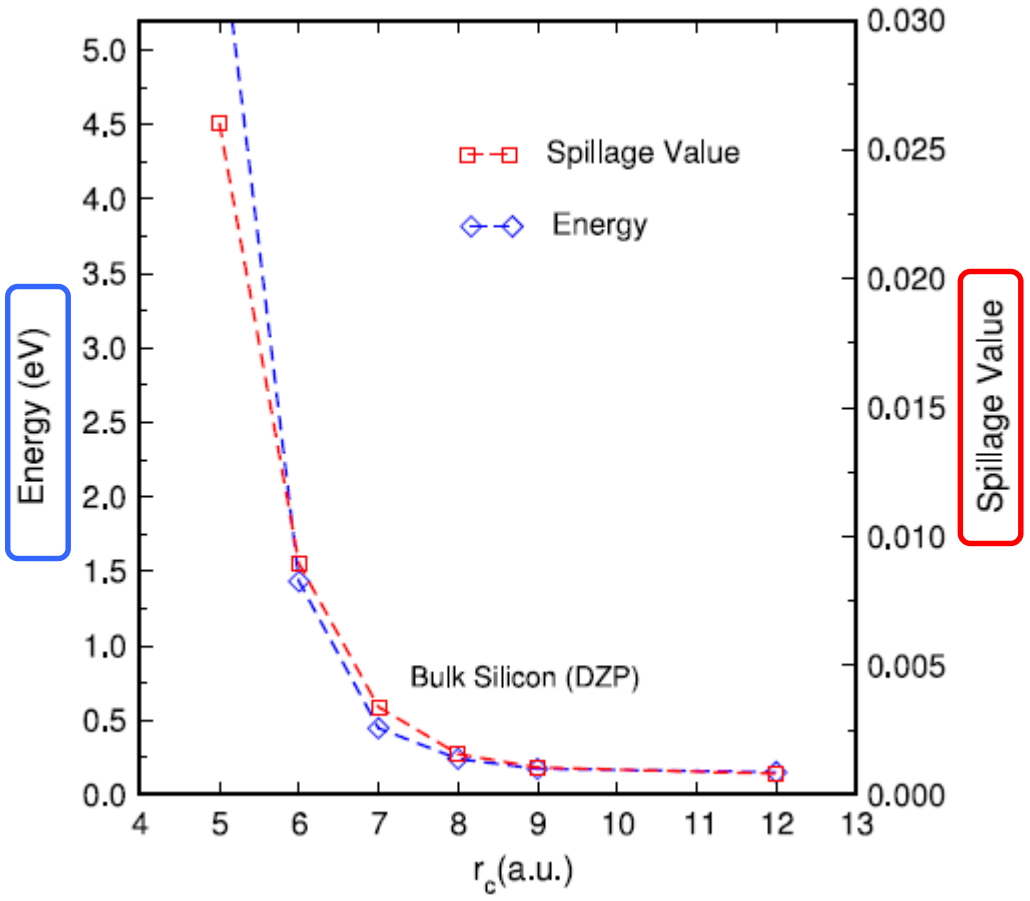
Spillage decreases

↓

Better atomic orbitals

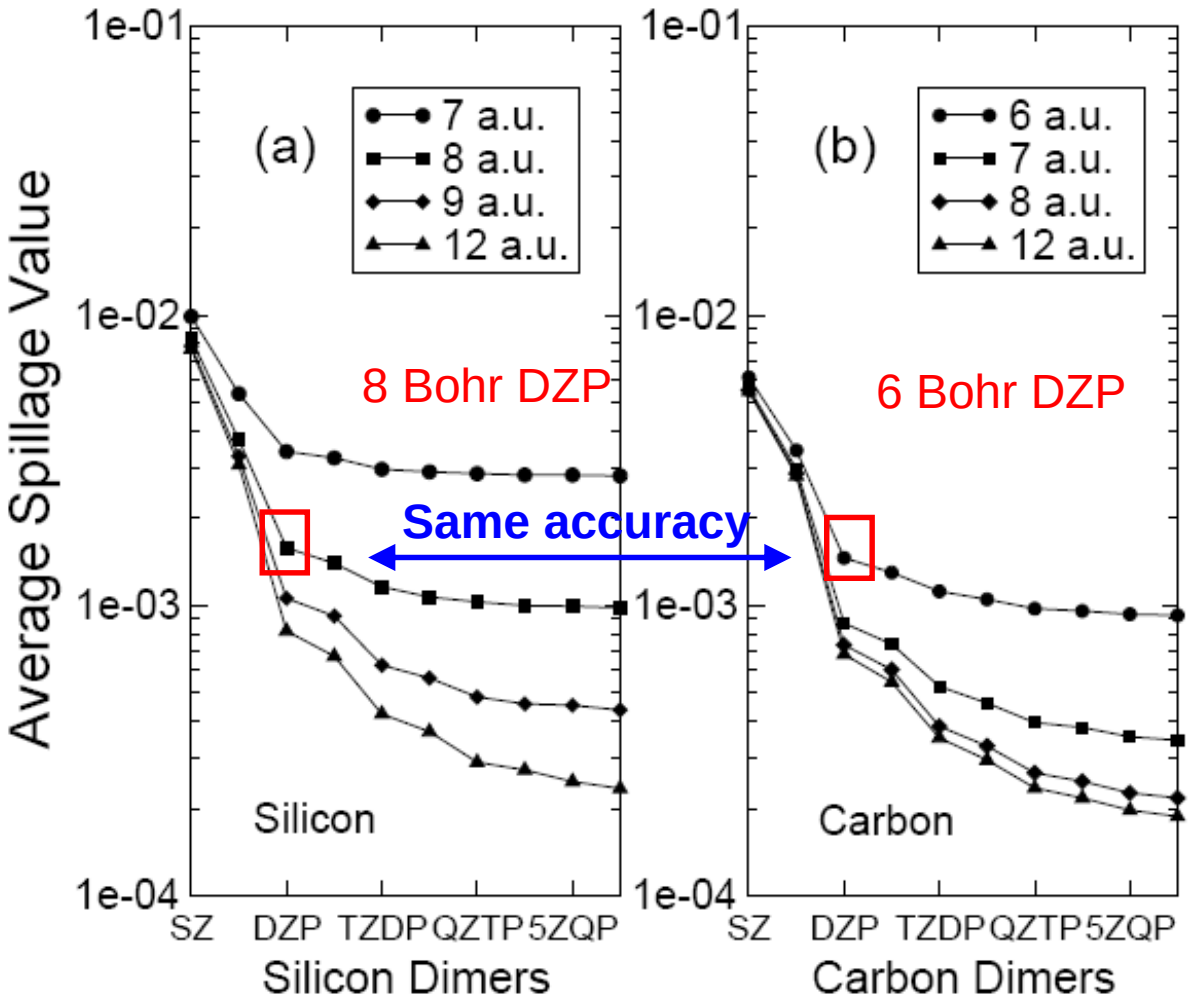
↓

Lower total energy



Spillage can describe very well the convergence of the total energy!

Balance the accuracy of different elements

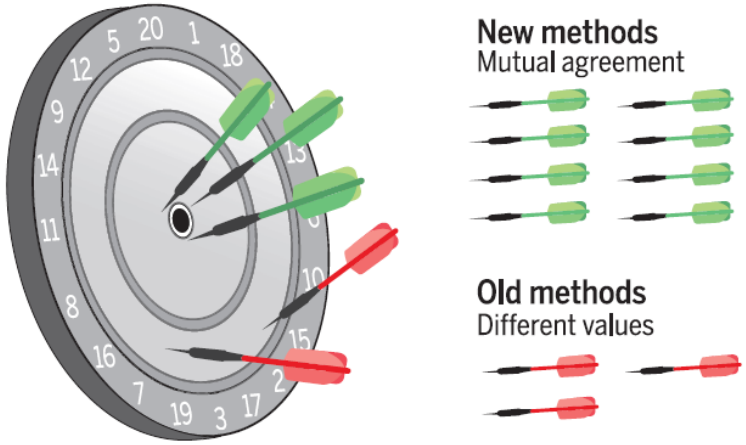


RESEARCH ARTICLE

DFT METHODS

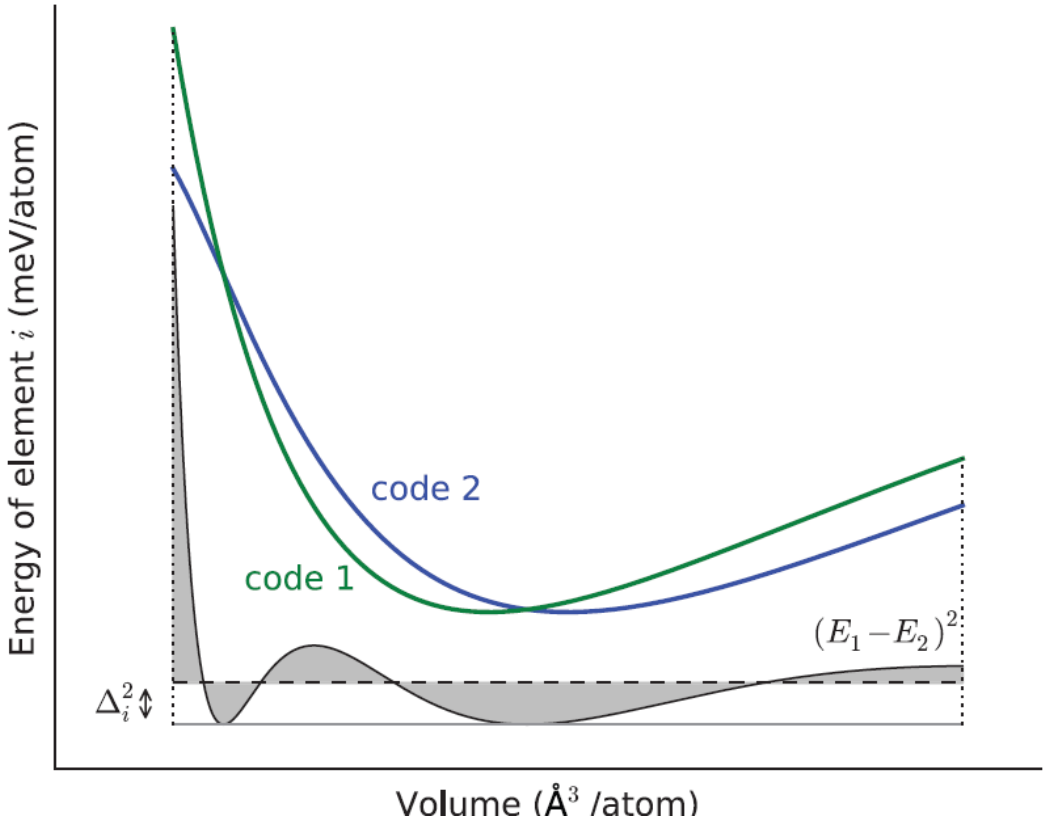
Reproducibility in density functional theory calculations of solids

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. Cl Andrea Dal Corso,[11] Stefano de Gironcoli,[11] Thierry Deutsch,[7,8] John Kay Dewhu 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 Lubec 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 Rignane 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*]



Stefaan Cottenier et al., Science **351**, 1415 (2016)

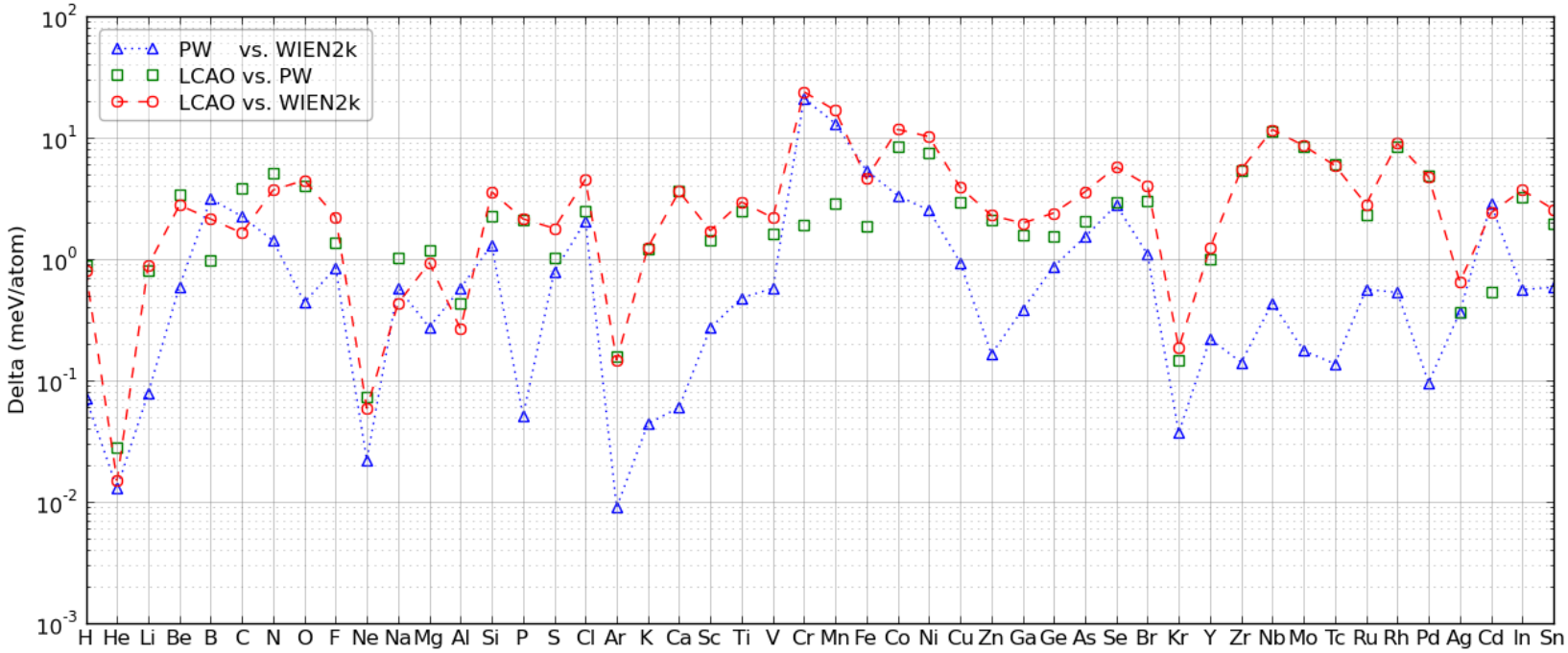
Fig. 3. Graphical representation of the Δ gauge. The black curve depicts the quadratic energy difference between two EOS [$(E_1 - E_2)^2$, where the subscripts correspond to the two codes shown], and Δ_i corresponds to the root-mean-square average. This is demonstrated by the shaded area, which is equally large above and below the Δ_i^2 line.



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

Stefaan Cottenier et al., Science **351**, 1415 (2016)

DZP bases



LCAO-DZP vs. PW $\langle\Delta\rangle \approx 2.9$ meV

LCAO-DZP vs. WIEN2K $\langle\Delta\rangle \approx 3.0$ meV

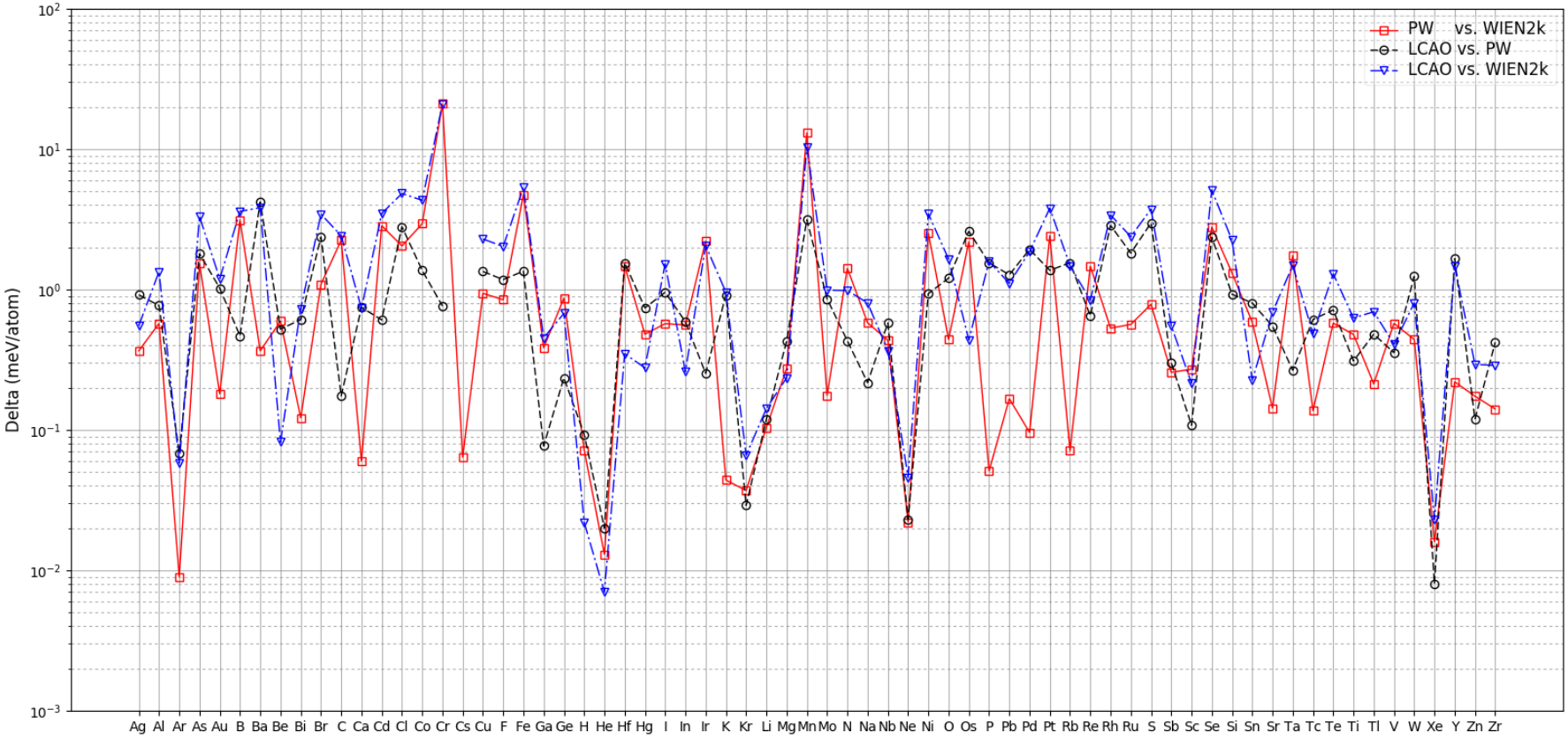
(no f orbitals for 3d, 4d elements)

NC(SG15) $\langle\Delta\rangle \approx 1.4$ meV

PAW $\langle\Delta\rangle \approx 0.6 - 1.6$ meV

USPP $\langle\Delta\rangle \approx 0.5 - 6.3$ meV

TZDP bases



LCAO-TDZP vs. PW $\langle \Delta \rangle \approx 0.9$ meV

LCAO-TDZP vs. WIEN2K $\langle \Delta \rangle \approx 1.9$ meV

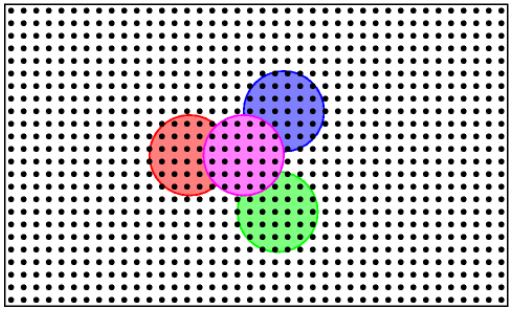
SG15 $\langle \Delta \rangle \approx 1.4$ meV

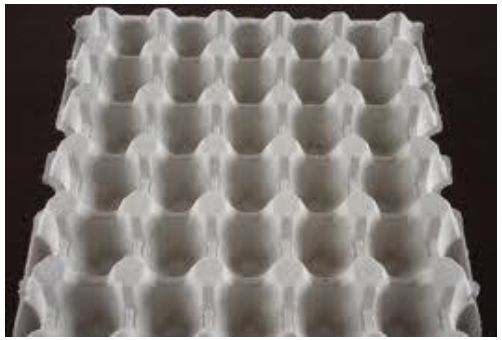
PAW $\langle \Delta \rangle \approx 0.6 - 1.6$ meV

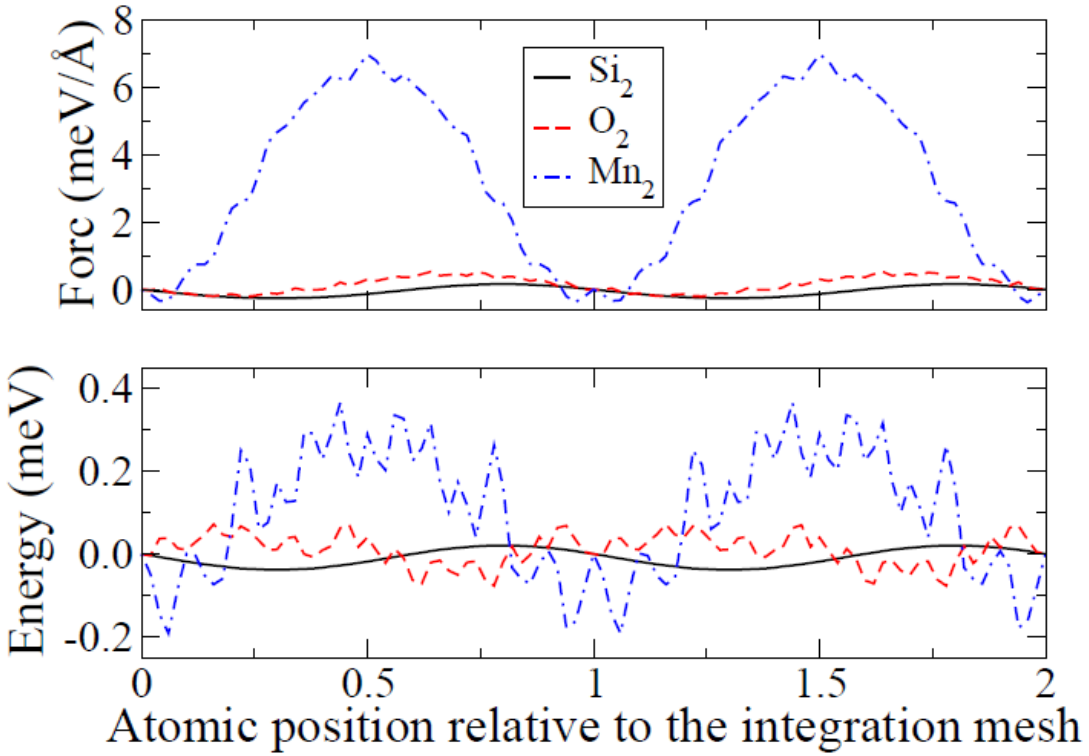
USPP $\langle \Delta \rangle \approx 0.5 - 6.3$ meV

Egg-Box effects

Translation symmetry broken by grid points!







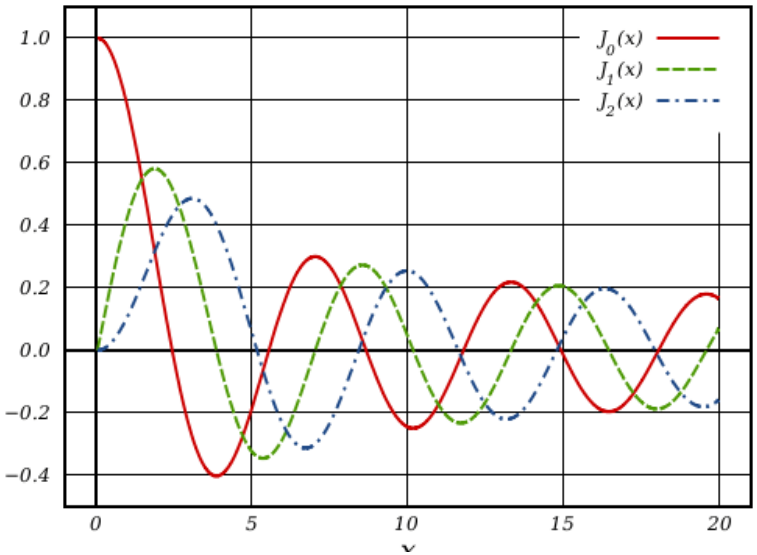
SIESTA used a special filtering procedure to reduce the egg-box effects

P-F Li et al. Computational Materials Science 112 (2016) 503–517

Egg-Box effects – why?

$$f_{\mu,l}(\mathbf{r}) = \begin{cases} \sum_q c_{\mu q} j_l(qr), & r < r_c \\ 0 & r \geq r_c \end{cases}$$

Spherical Bessel functions:



Strictly Localized orbitals usually have high **G** components, resulting in egg box effects.

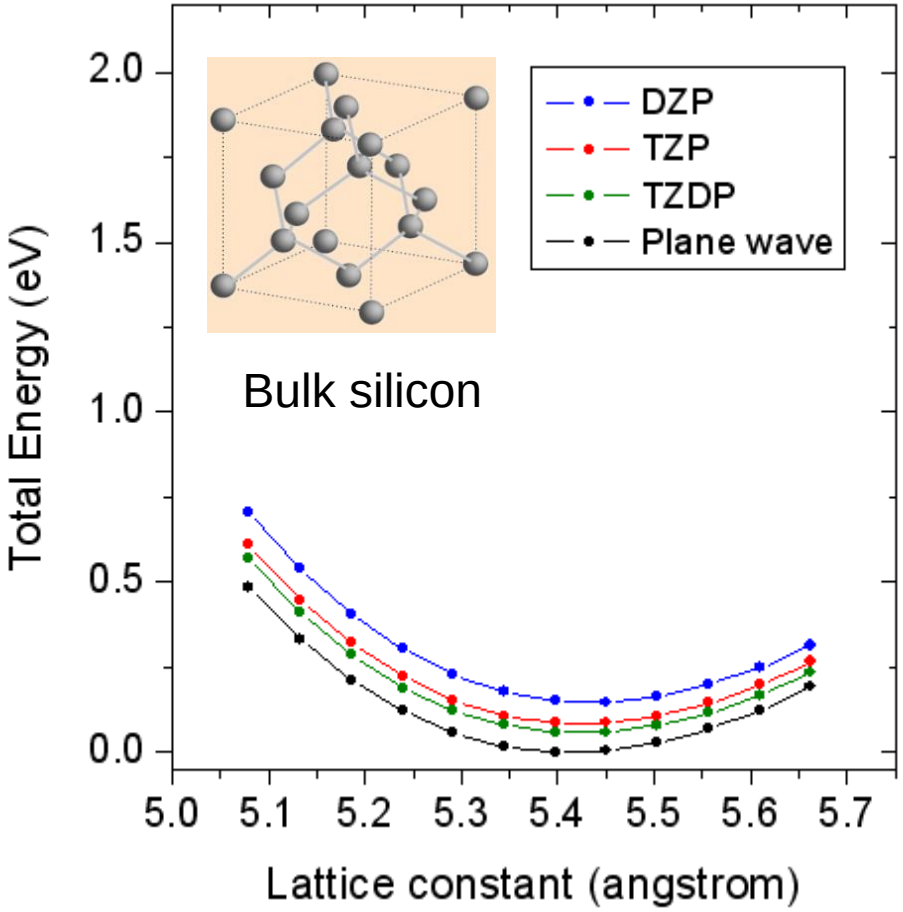
Our scheme allow the atomic orbitals localized both in real space and in **G** space!

Tested Systems

- ✓Molecules
  - Bond length, vibration frequency, atomization energy
- ✓Solid (bulk)
  - Lattice constants, cohesive energy, bulk modulus, structure
- ✓Surface reconstruction

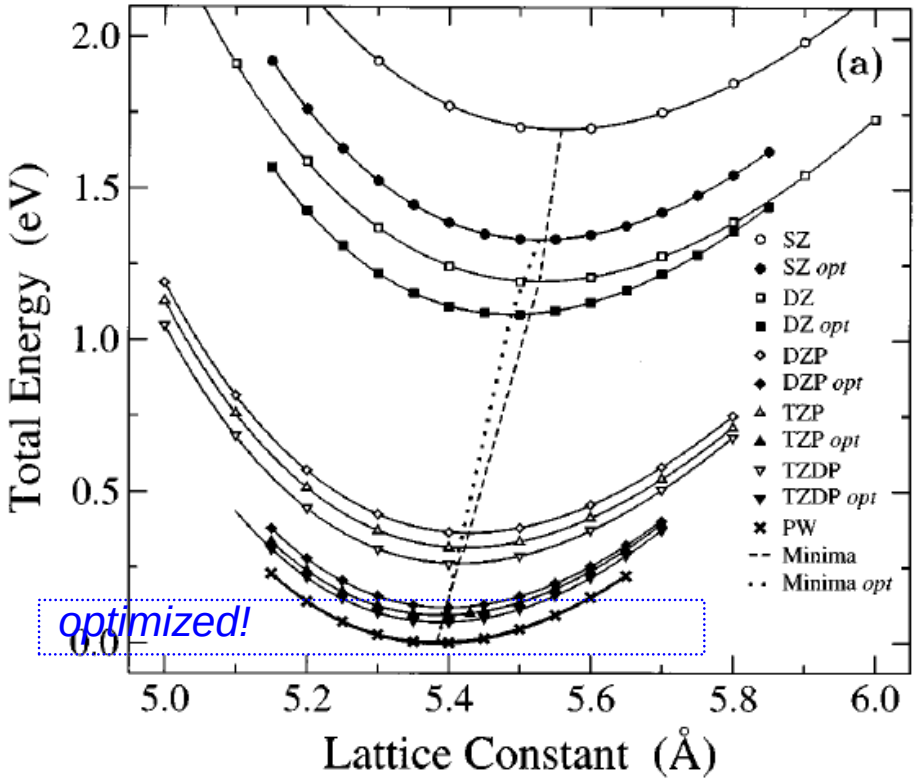
Test on bulk Si

Our orbitals



◆References: dimers

SIESTA



◆ references: bulk Si。

J. Junquera et al, Phys Rev B **64**, 235111 (2001)

Semiconductors

Compound	a SZ	DZP	TZDP	PW	Expr.	B SZ	DZP	TZDP	PW	Expr.
GaAs	10.67	10.50	10.49	10.48	10.68[a]	69	78	77	77	75.57[c]
GaP	10.28	10.11	10.11	10.10	10.30[a]	82	92	93	93	89[d]
GaSb	11.54	11.38	11.37	11.36	11.52[a]	49	59	58	57	57[d]
InAs	11.40	11.27	11.28	11.28	11.45[a]	63	66	65	65	60[d]
InP	11.07	10.94	10.94	10.93	11.09[a]	78	79	79	80	71[d]
InSb	12.33	12.05	12.05	12.07	12.24[a]	41	50	49	50	47[d]
AlAs	10.88	10.63	10.62	10.59	10.70[a]	67	76	76	76	77[d]
AlP	10.50	10.26	10.25	10.21	10.33[a]	64	87	88	89	86[d]
AlSb	11.83	11.58	11.57	11.54	11.59[a]	48	55	56	56	58[d]
Ge	10.82	10.68	10.61	10.61	10.70[c]	57	67	71	71	77.20[c]
Si	10.59	10.28	10.25	10.23	10.26[b]	74	94	94	94	99[b]
C[e]	6.78	6.67	6.67	6.67	6.75[b]	436	470	467	466	442[b]

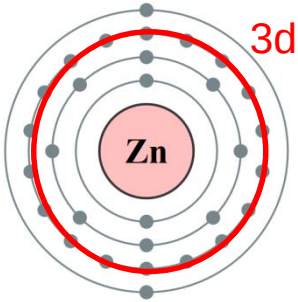
晶格常数平均误差(Bohr) : 0.218 (SZ), 0.026 (DZP), 0.015 (TZDP)

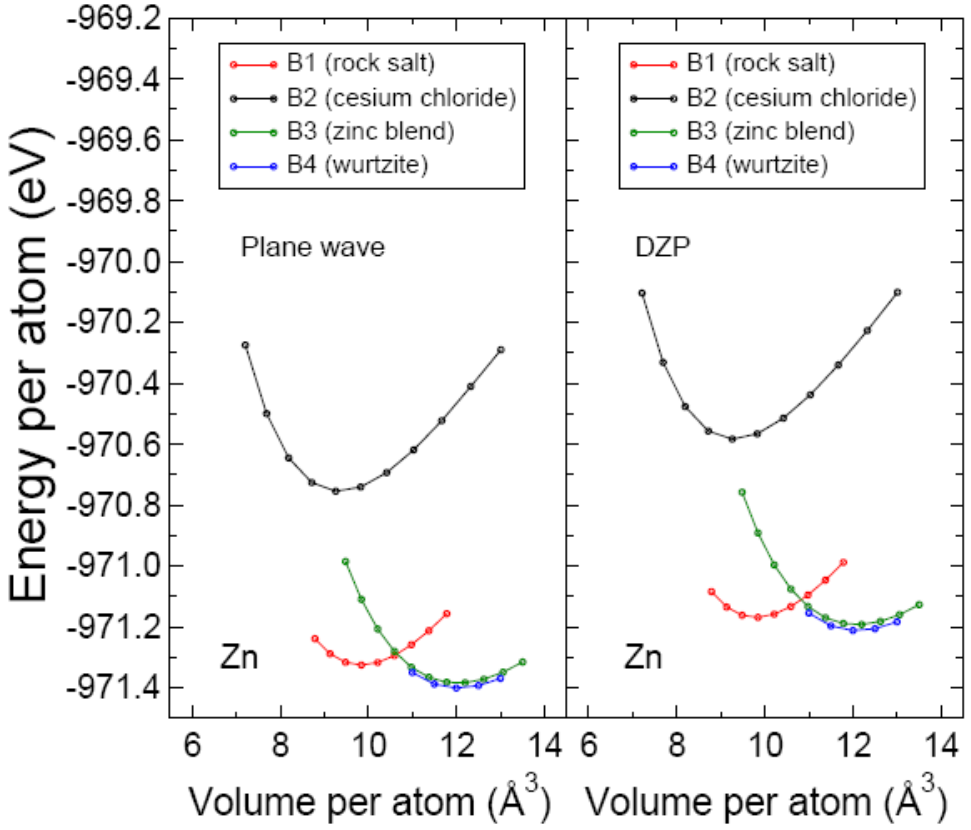
体弹性模量平均误差(GPa) : 12.3 (SZ), 1.4 (DZP), 0.4 (TZDP)

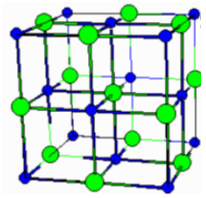
DZP 可以准确预测半导体的结构性质

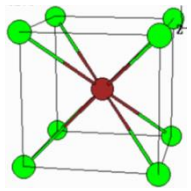
Tests on ZnO

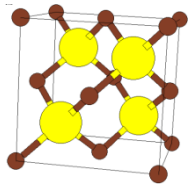
- Include 3d electrons
- Four phases

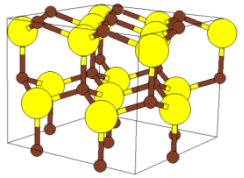





B1 (NaCl)


B2 (CsCl)


B3 (Zinc Blend)

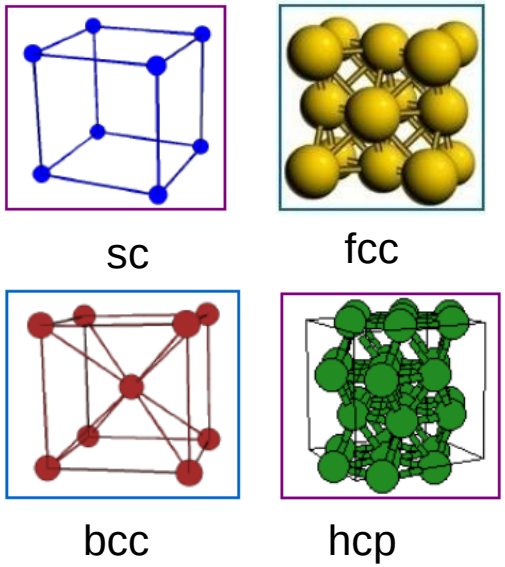

B4 (Wurtzite)

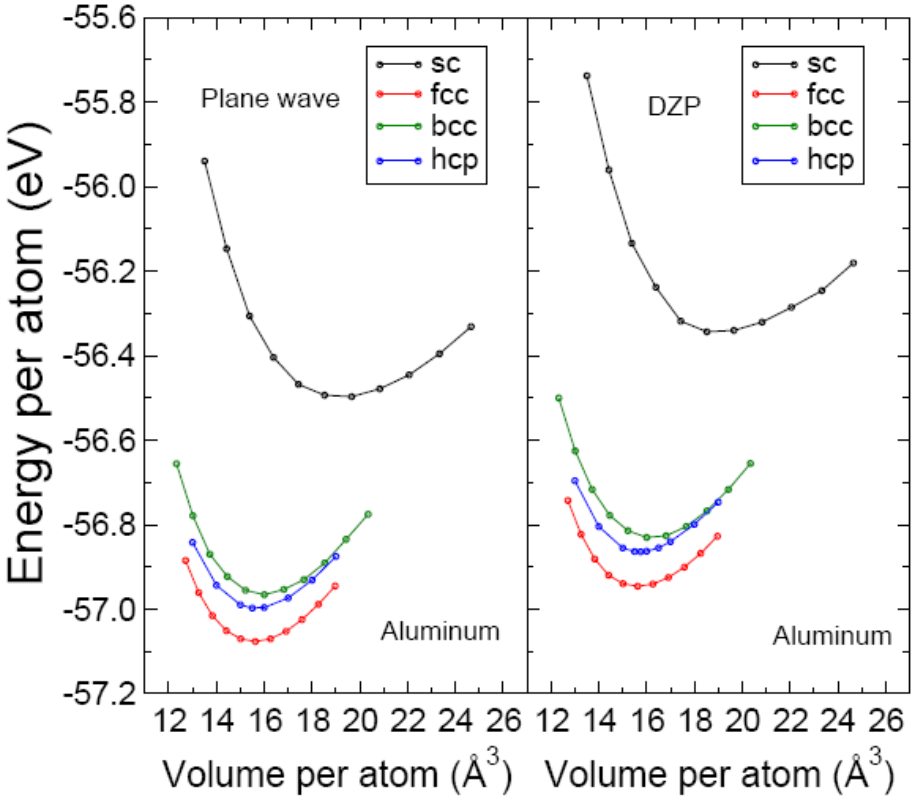
Correct energy orders and energy differences!

Good transferability !

Tests on Al (metal)

- Metal
- Four different structures





Correct energy orders and energy differences!

LCAO works well for metals and insulators。

Electronic structure interpolation via atomic orbitals

Mohan Chen, G-C Guo, and **Lixin He**, *J. Phys.: Cond. Mat.* **23** 325501 (2011)

Motivation : Large k sampling problem

The number of k points used to calculate anomalous Hall conductivity in bcc Fe:

Self consistent – 20, 000 k points

Berry curvature , larger than 400,000 – 2,000,000 k points

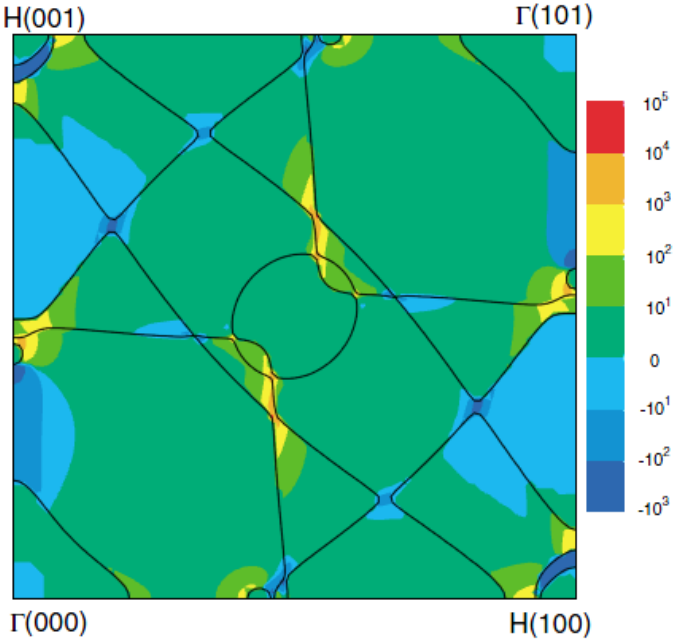
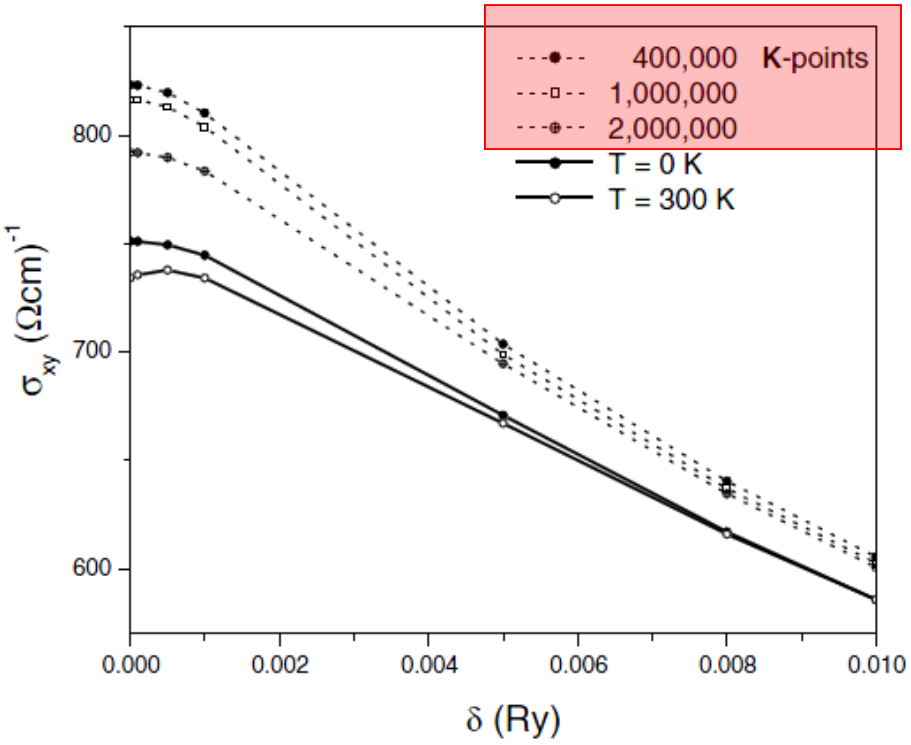


FIG. 3 (color). Fermi surface in (010) plane (solid lines) and Berry curvature $-\Omega^z(\mathbf{k})$ in atomic units (color map).



Yugui Yao et al, Phys. Rev. Lett **92**, 037204 (2004)

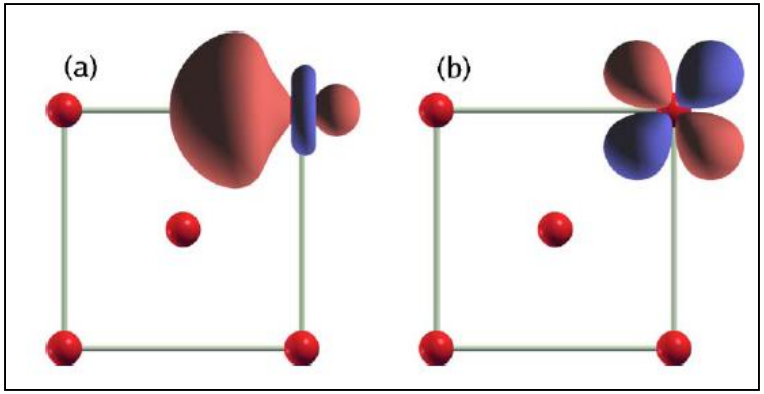
First Principle Calculation of Anomalous Hall Conductivity in Ferromagnetic bcc Fe

Band interpolation via Wannier functions

- Maximally localized wannier functions (MLWF)

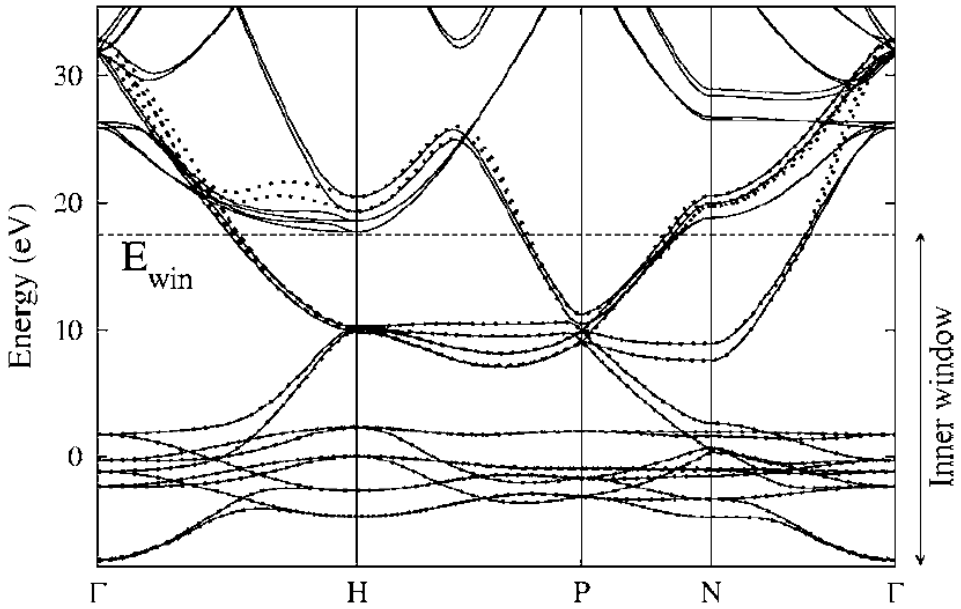
Minimize the spread functional:

$$\Omega = \sum_n \left[\langle r^2 \rangle_n - \overline{\mathbf{r}}_n^2 \right]$$



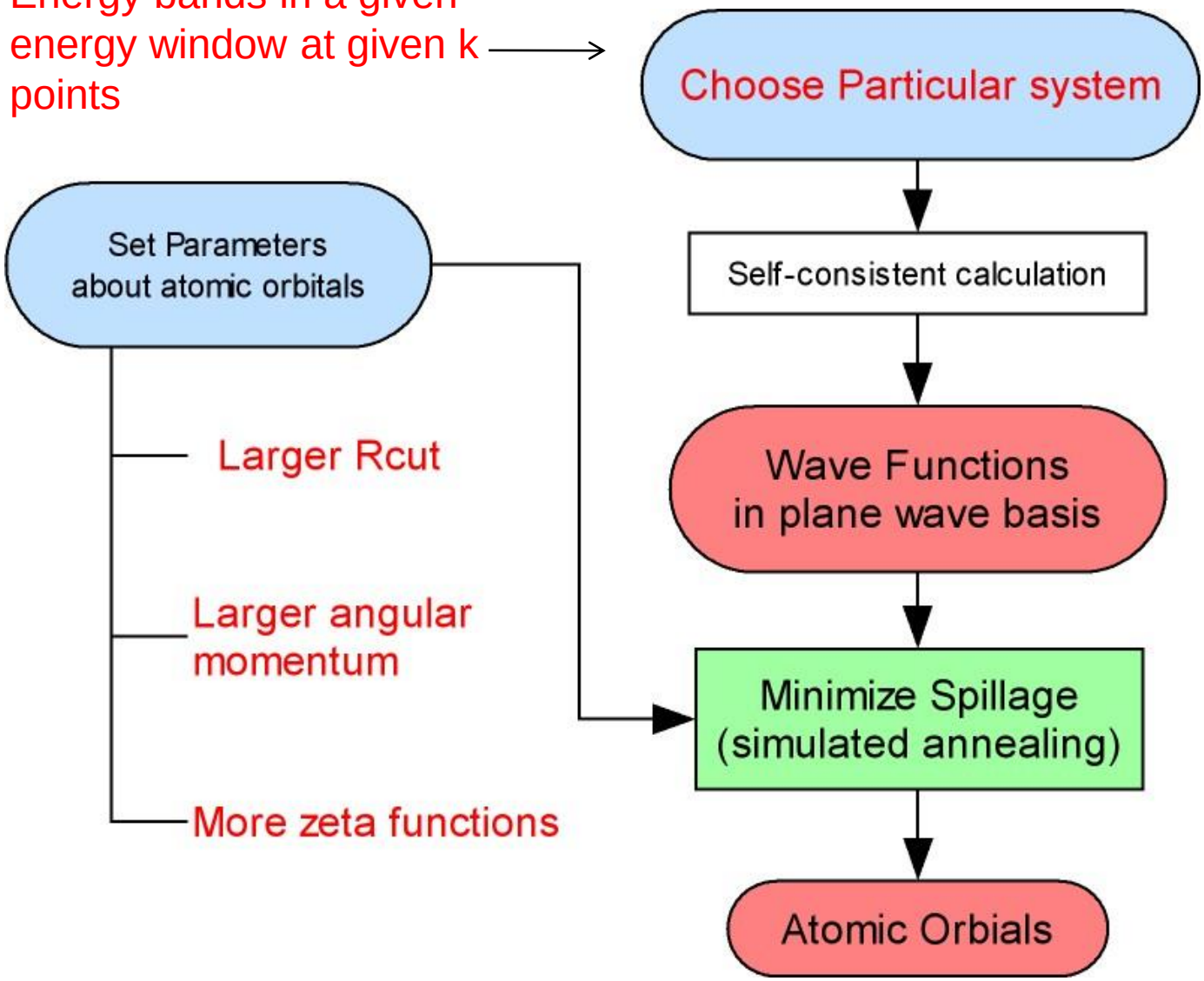
MLWF

Band structure of bcc Fe



Xinjie Wang et al, Phys. Rev. B **74**, 195118 (2006)

Our Method: atomic basis



Interpolation of operators

$$H_{\mu\nu}(\mathbf{R_n}) = \langle \phi_{\mu 0} | \hat{H} | \phi_{\nu \mathbf{n}} \rangle,$$

Calculate once for all k-points

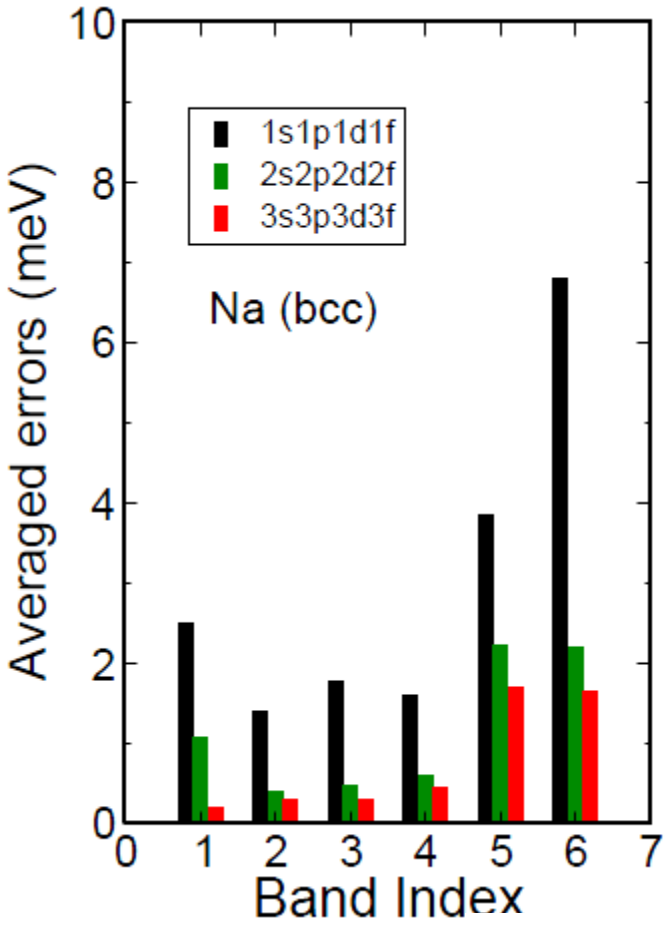
$$H_{\mu\nu}(\mathbf{k}) = \sum_{\mathbf{R_n}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R_n}} H_{\mu\nu}(\mathbf{R_n}),$$

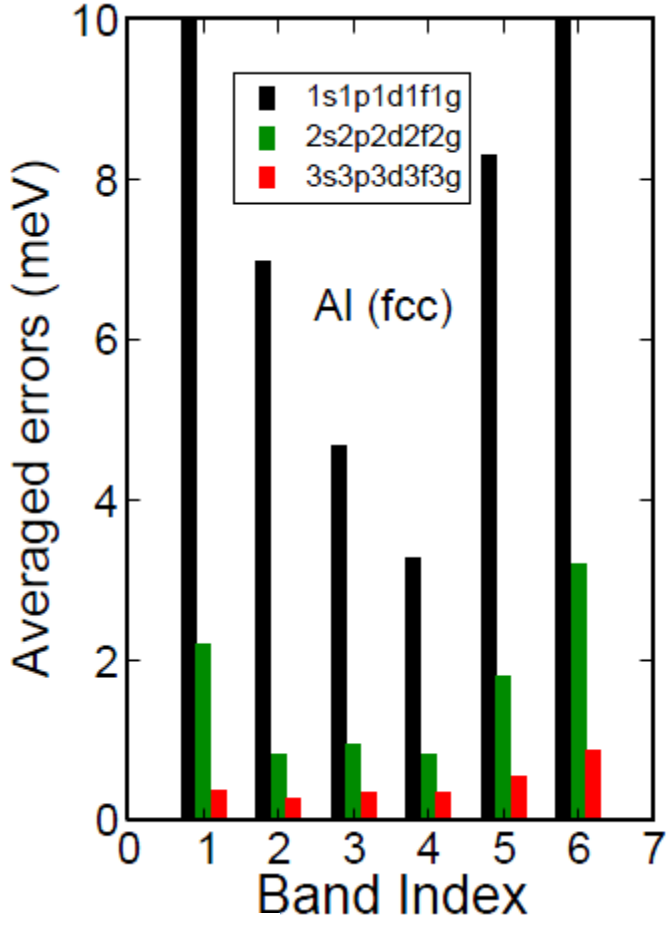
$$\Psi_{i\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R_n}} c_{i\mu}(\mathbf{k}) \phi_\mu(\mathbf{r} - \mathbf{r}_\mu - \mathbf{R_n}) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R_n}}.$$

$$O_{ij}(\mathbf{k},\mathbf{q}) = \left\langle \psi_{i,\mathbf{k}} \left| \hat{O} \right| \psi_{j,\mathbf{q}} \right\rangle$$

$$O_{ij}(\mathbf{k}, \mathbf{q}) = \sum_{\mathbf{R_n}\mathbf{R_m}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R_n} + \mathrm{i}\mathbf{q}\cdot\mathbf{R_m}} c^*_{i\mu}(\mathbf{k}) c_{j\nu}(\mathbf{q}) \langle \phi_{\mu \mathbf{n}} | \hat{O} | \phi_{\nu \mathbf{m}} \rangle.$$

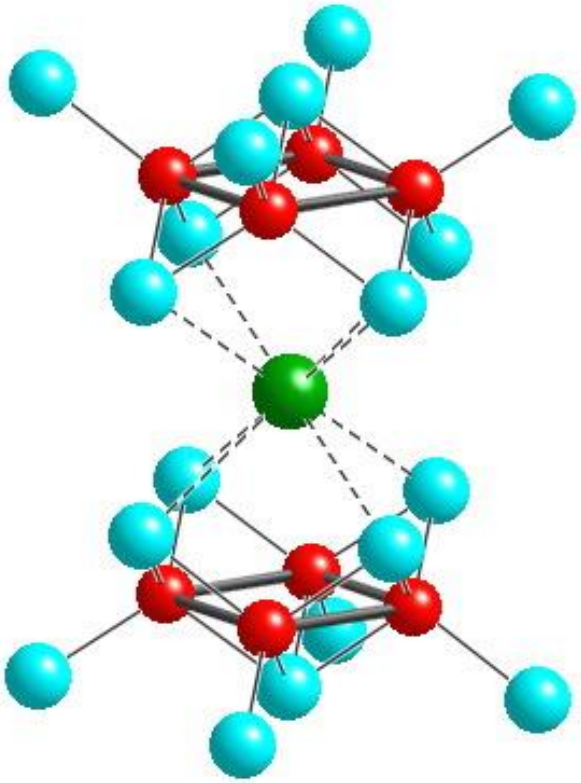
Test: Na (bcc) , Al (fcc)

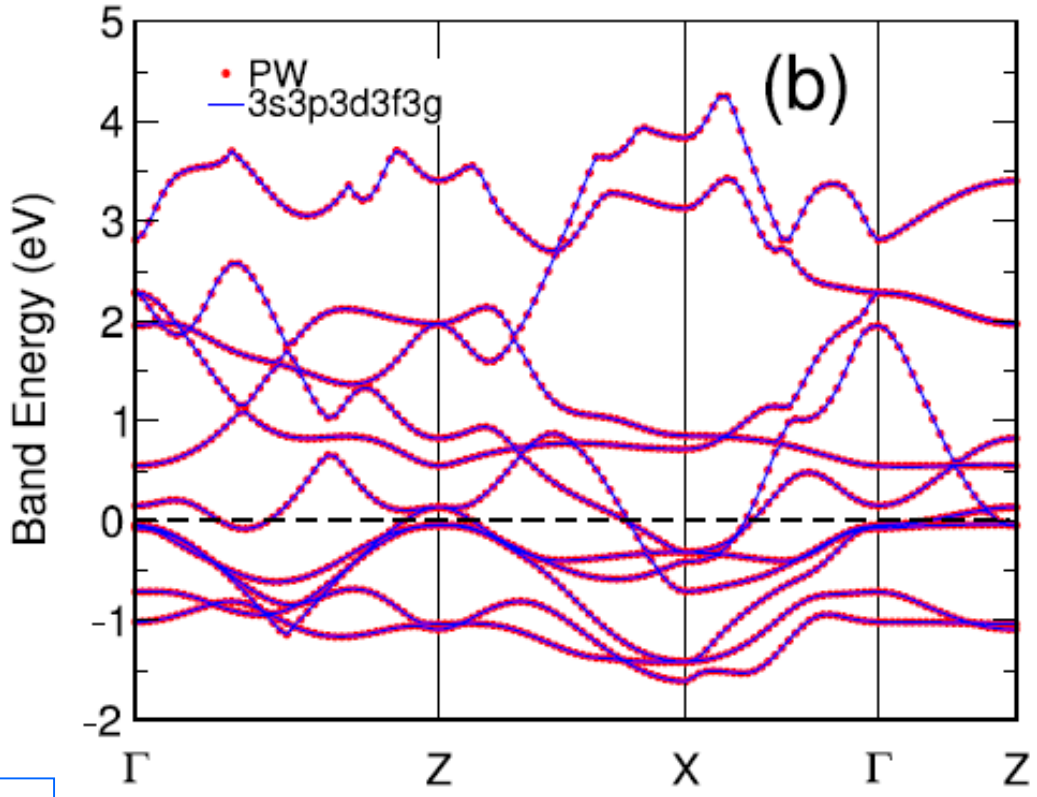




$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{N} \frac{(\epsilon_i^{\mathrm{PW}} - \epsilon_i^{\mathrm{LCAO}})^2}{N}},$$

Test: $BaFe_2As_2$





平面波: 5319
1s1p1d1f1g: 125(快884倍)
2s2p2d2f2g: 250 (快212倍)
3s3p3d3f3g: 375 (快81倍)

2s2p2d2f2g is accurate enough! (< 3meV)

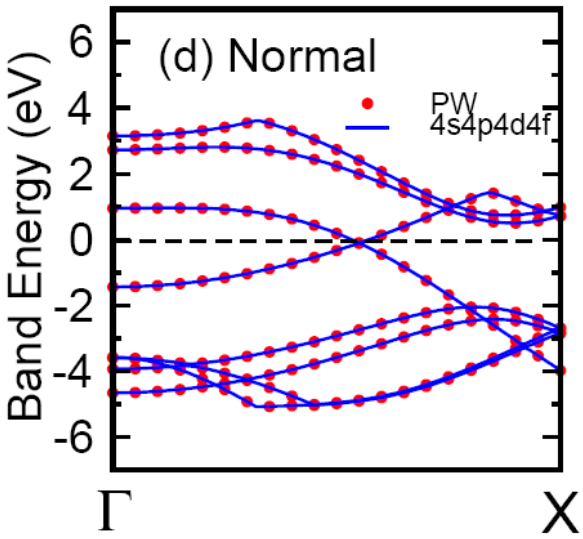
Mohan Chen, G-C Guo, and **Lixin He**, *J. Phys.: Cond. Mat.* **23** 325501 (2011)

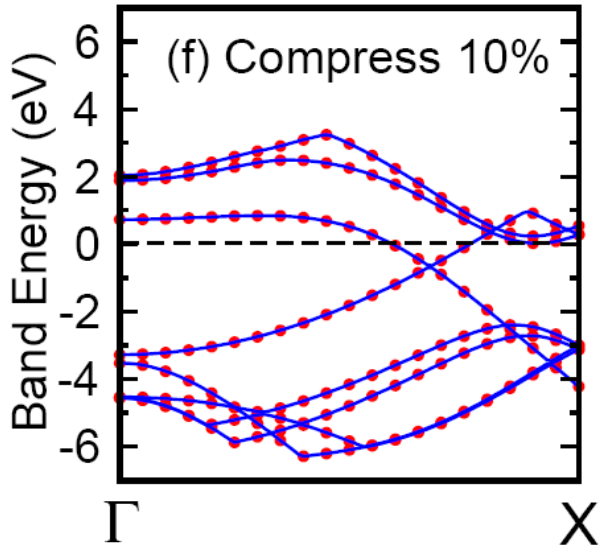
Transferability of the bases

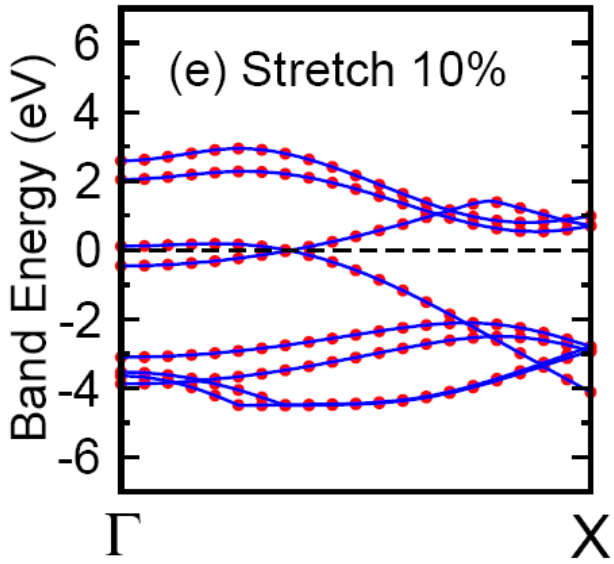
◆ Atomic orbitals generated under normal conditions (10 Bohr, 4s4p4d4f)

planewaves: 17221
Atomic bases(4s4p4d4f): 768

Compressed by 10%



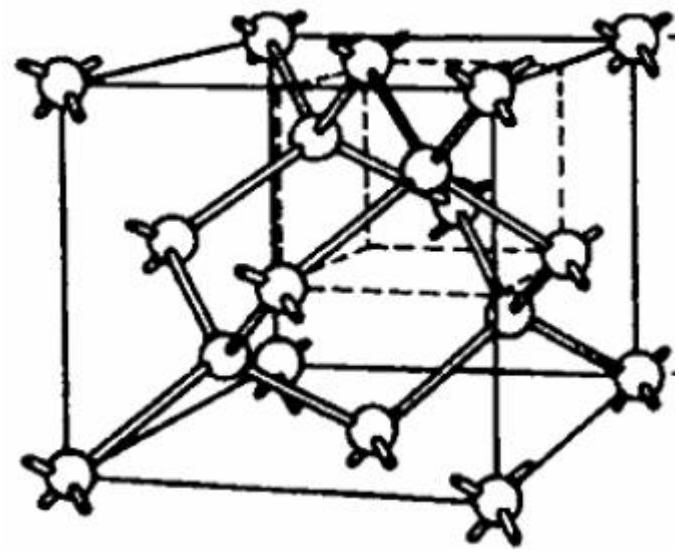


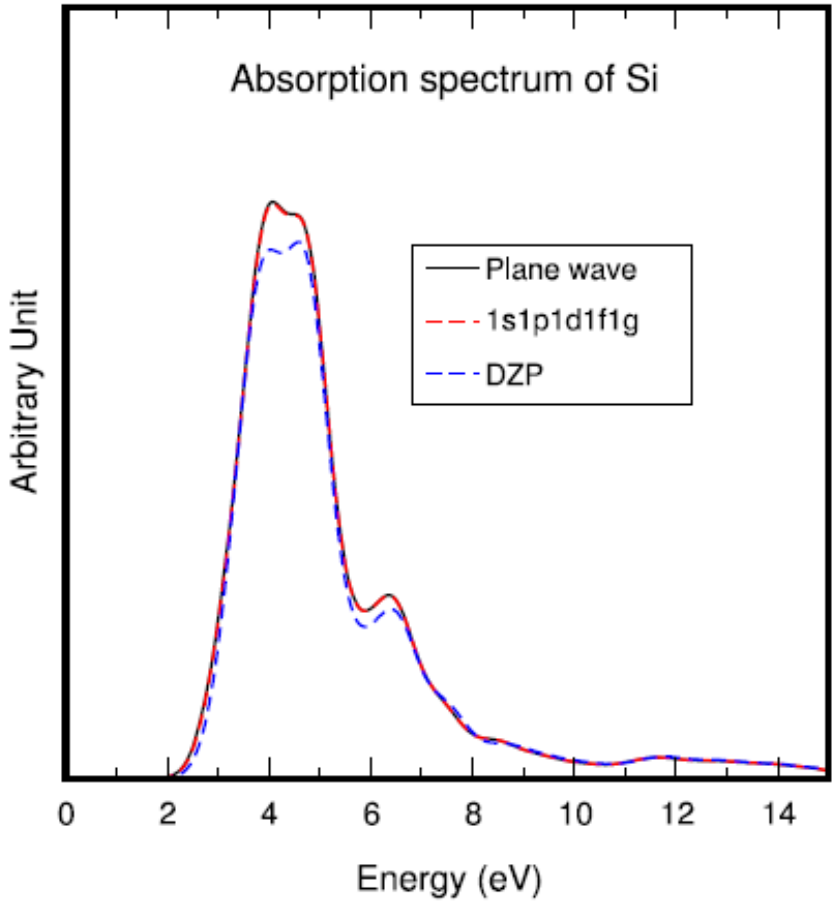


Stretched by 10%

Good transferability!

Absorption spectrum of Si





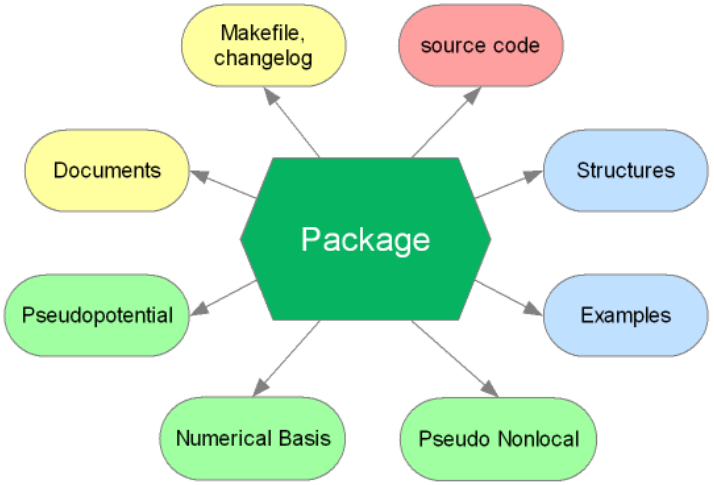
xc：LDA
K points：13*13*13

Dielectric function：

$$\epsilon_2(\omega) = \frac{2e^2\pi}{\Omega\epsilon_0} \sum_{\mathbf{k},c,v} |\langle \Psi_{\mathbf{k},c} | \hat{\mathbf{e}} \cdot \mathbf{r} | \Psi_{\mathbf{k},v} \rangle|^2 \delta\left[E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega \right]$$

ABACUS project

- Atomic-orbital Based Ab-initio Computation at USTC
- Written in C++
- Start at 2007
- first version v1.0.0 released at 2015.10
- v1.0.1 released at 2016.12
- v1.1 will be released in 2018



http://abacus.ustc.edu.cn/

http://abacus.ustc.edu.cn

ABACUS

ATOMIC-ORBITAL BASED AB-INITIO COMPUTATION AT USTC

Today is: Tuesday the 10th of October, 2017

News

16.12.19

ABACUS V1.0.1

ABACUS version1.0.1 is updated for download!

ABACUS (Atomic-orbtial Based Ab-initio Computation at UStc) is an open-source computer code package aiming for large-scale electronic-structure simulations from first principles, developed at the Key Laboratory of Quantum Information, University of Science and Technology of China (USTC) - C-omputer Network and Information Center, Chinese of Academy (CNIC of CAS).

.

ABACUS currently provides the following features and functionalities:

1.Ground-state total energy calculations using Kohn-Sham (KS) density functional theory (DFT) with local-density or generalized gradient approximations (LDA/GGAs).
2.Brillouin zone sampling using the Monkhorst-Pack special k-points.
3.Geometry relaxation with both Conjugated Gradient (CG) and BFGS methods.
4.Semi-emperical van der Waals energy correction using the Grimme DFT-D2 scheme.
5. NVT molecular dynamics simulation using the Nose-Hoover thermostat.

More about >>

 user's guide

 **pseudopotential library**

download

已完成

- Plane waves/Atomic orbital dual bases sets
- Normal conserving pseudopotential (UPF format)
- Functionals: LDA, GGA, spins, van der Waals (DFT-D2)
- Electronic structures，structural relaxation
- Molecular dynamics (NVE，NVT)

测试中

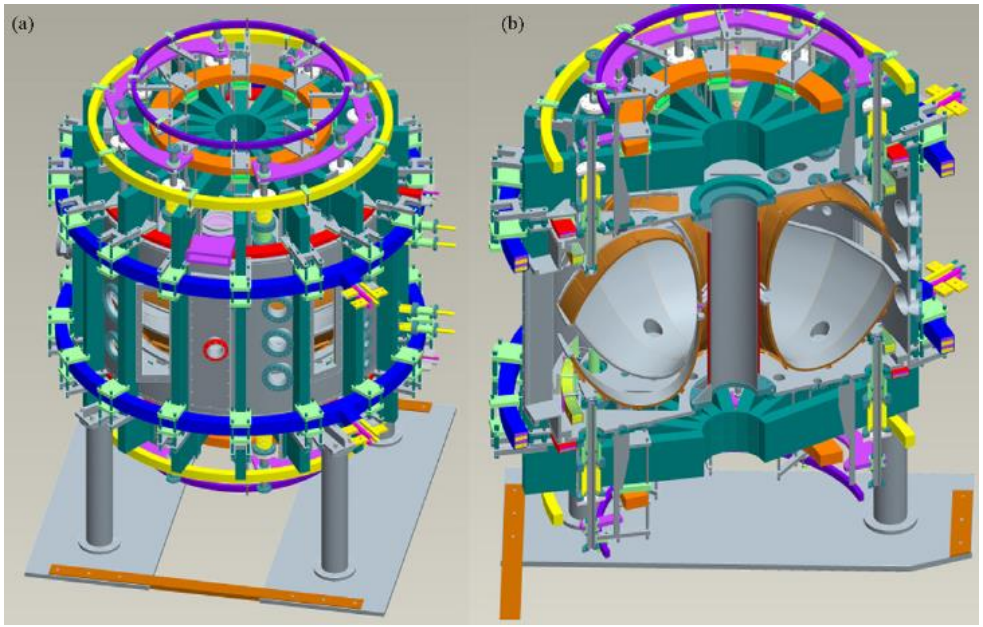
- stress and cell optimization
- Real-time TDDFT (cooperate with 孟胜）
- Berry phase
- Interface to Wannier90
- spin-orbital coupling
- Hybrid functional (HSE and PBE0)

Will be included in the next release

进行中

- RPA, GW, optical properties
- Transports (cooperate with 夏柯，袁喆）

Example: LiSn metal liquid



Lithium Tokamak Experiment (LTX),
Princeton Plasma Physics Laboratory (PPPL)

Liquid metals: promising materials are
lithium, tin, gallium, etc.

Advantages:

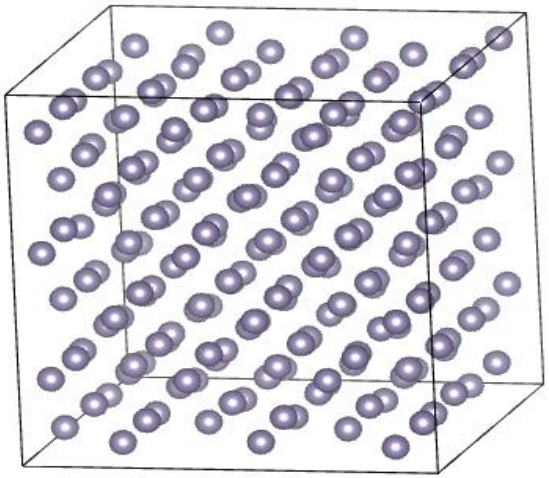
no irreversible erosion
no neutron damage
no heat overload

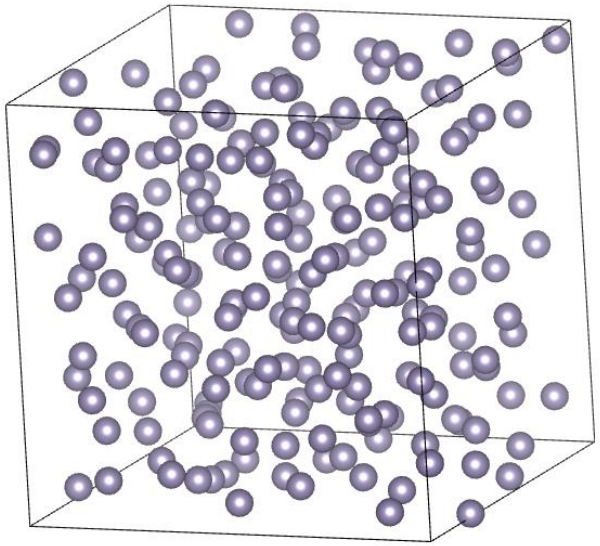
Nuclear fusion rector wall protection materials

MD simulation system size： 200 – 500 atoms

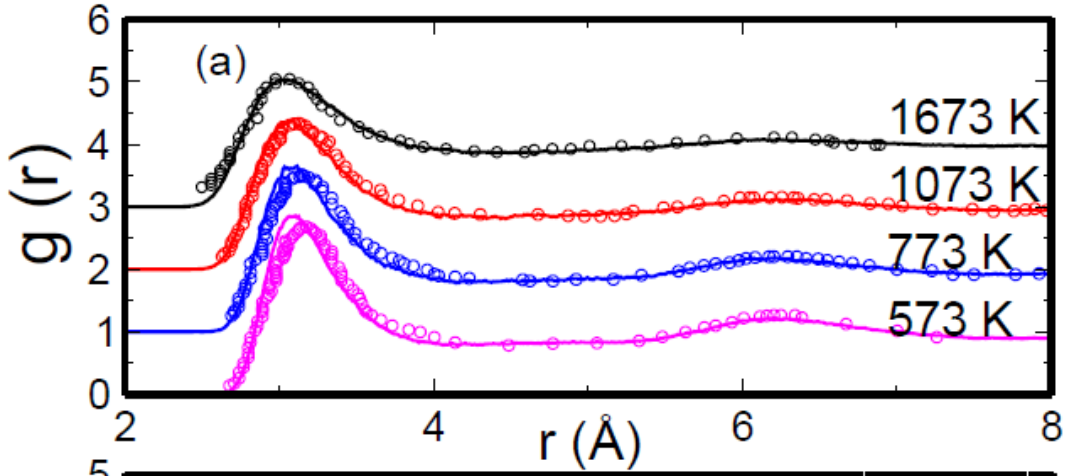
Structure properties of solid tin

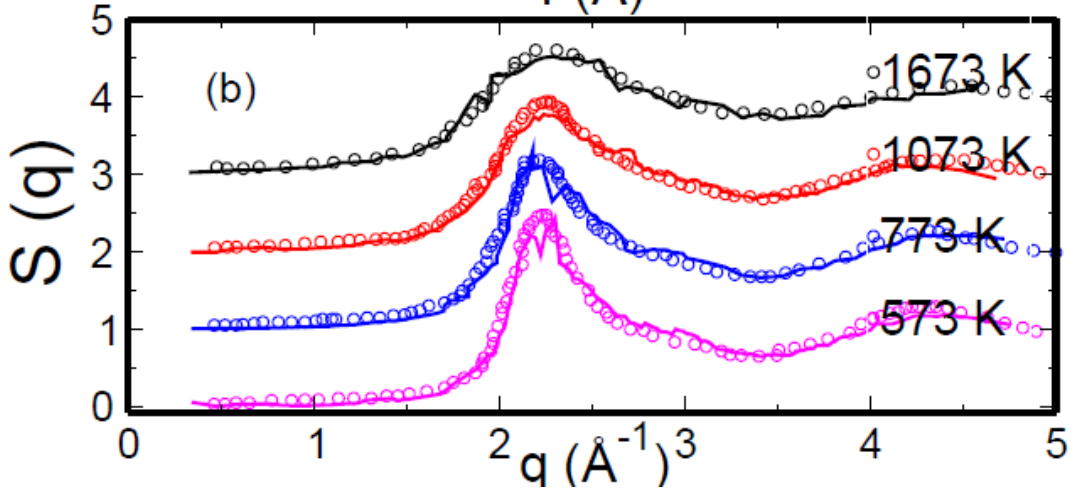
	a_0	c_0/a_0	V_0	ΔE	B_0	Method
β-tin	5.780	0.537	26.15	0.000	58	FP (PW)
	5.786	0.538	26.23	0.000	57	FP (LCAO)
	5.831	0.546	27.07	-	-	EXP[45]
	5.8119	0.543	26.65	-	-	EXP[46]
	-	-	-	-	57.037	EXP[47]
	-	-	-	-	57.9	EXP[48]
α-tin	6.442	-	33.41	-0.019	43	FP (PW)
	6.445	-	33.47	-0.055	43	FP (LCAO)
	6.483	-	34.05	-	-	EXP[45]
	-	-	-	-	42.617	EXP[47]
	-	-	-	-	54	EXP[49]
bct	3.933	0.846	25.73	0.045	53	FP (PW)
	3.920	0.844	25.42	0.047	54	FP (LCAO)
bcc	3.664		24.60	0.095	70	FP (PW)
	3.658		24.47	0.130	71	FP (LCAO)





$$g(r) = \frac{1}{\rho N}\langle \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} \delta(\mathbf{r} - \mathbf{R}_i + \mathbf{R}_j)\rangle$$

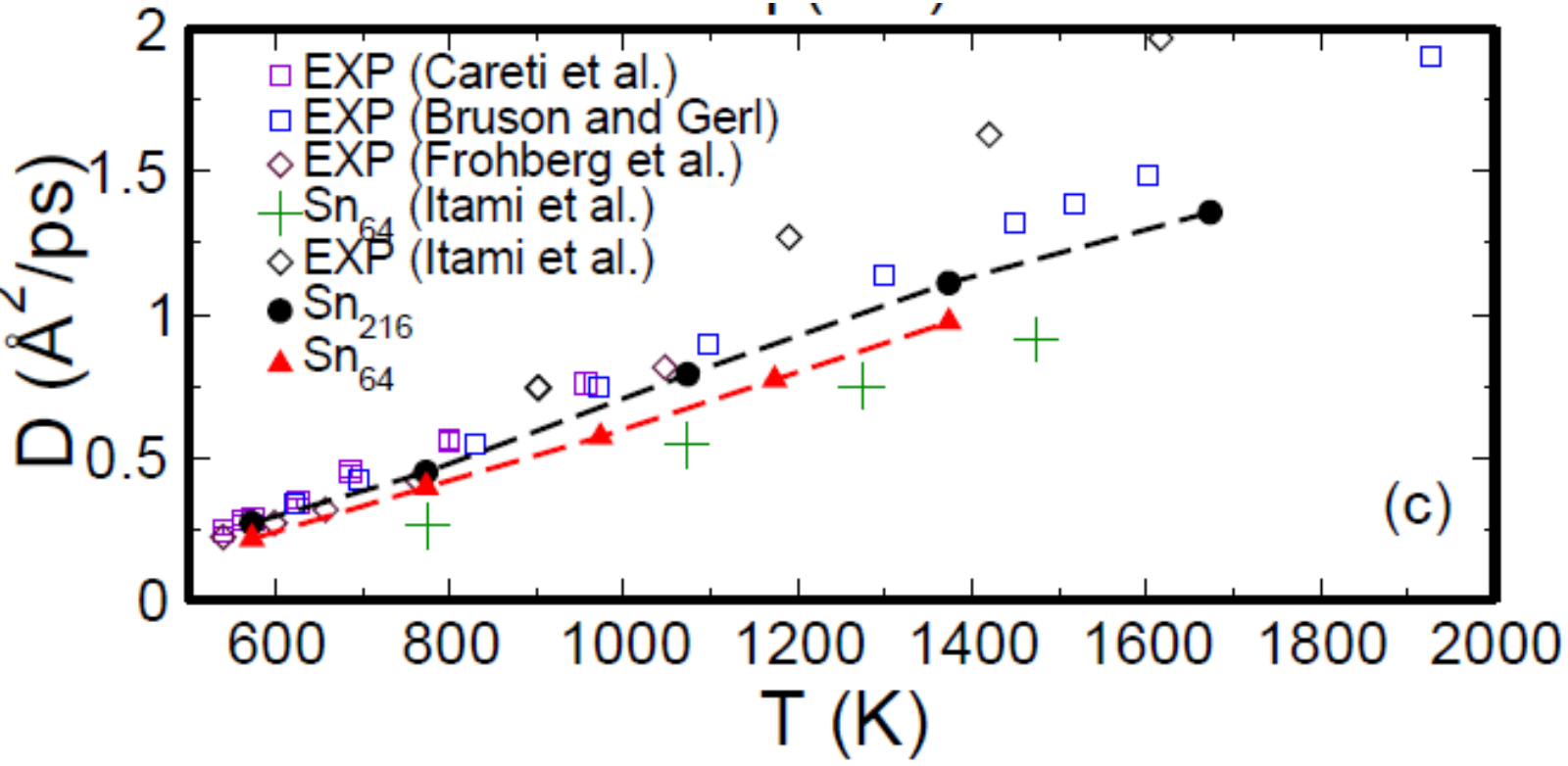




$$S(q) = \frac{1}{N}\langle \sum_{i=1}^{N} \sum_{j=1}^{N} e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}\rangle$$

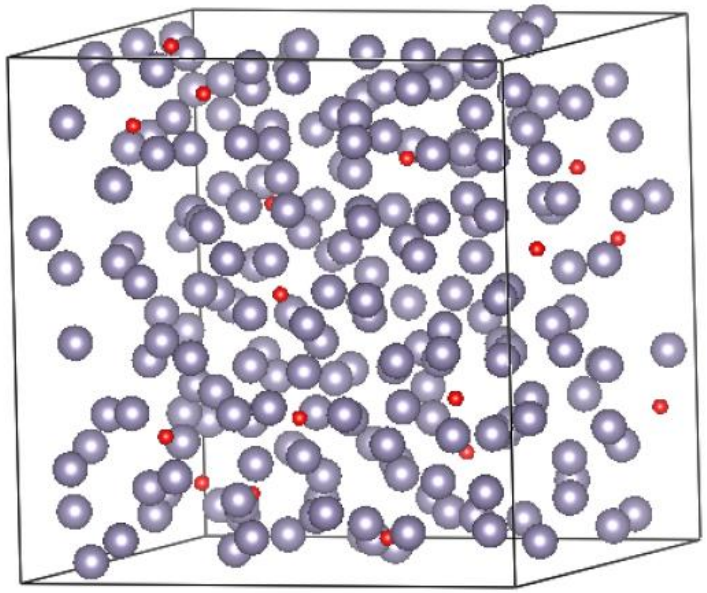
216 atoms, 32 cores, ~30 s/MD step

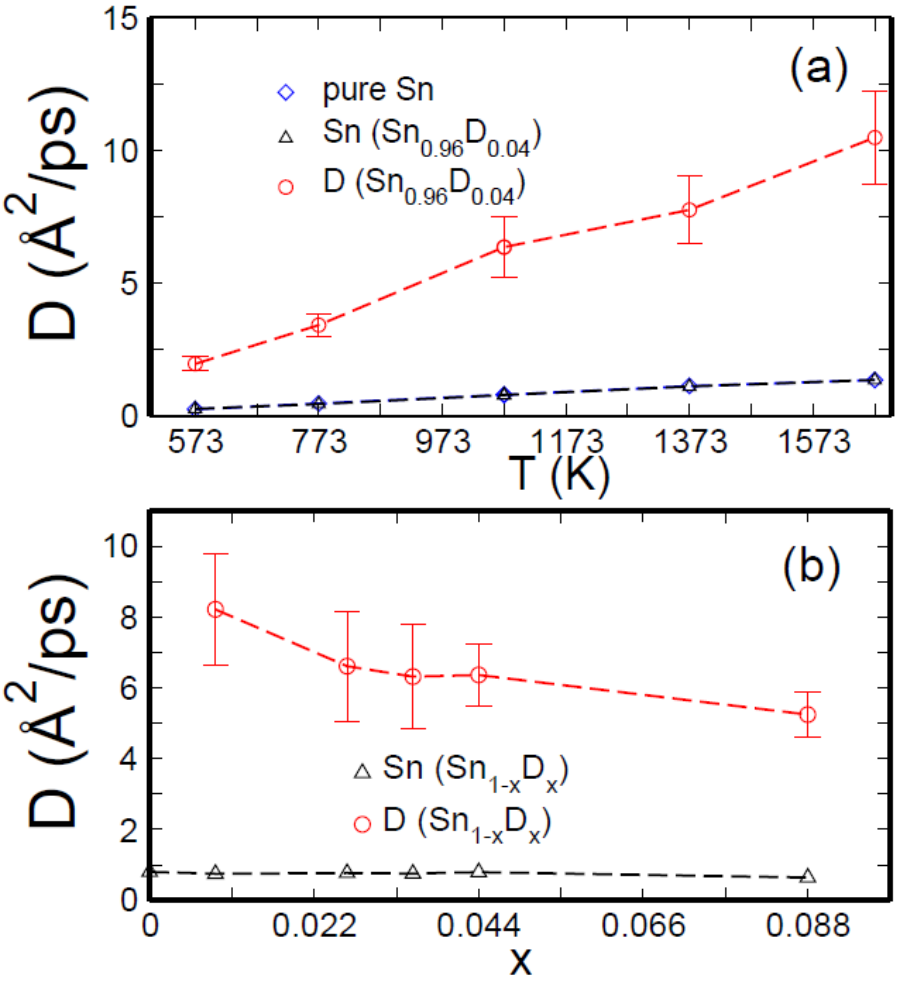
Diffusion coefficient of pure Sn metal liquid



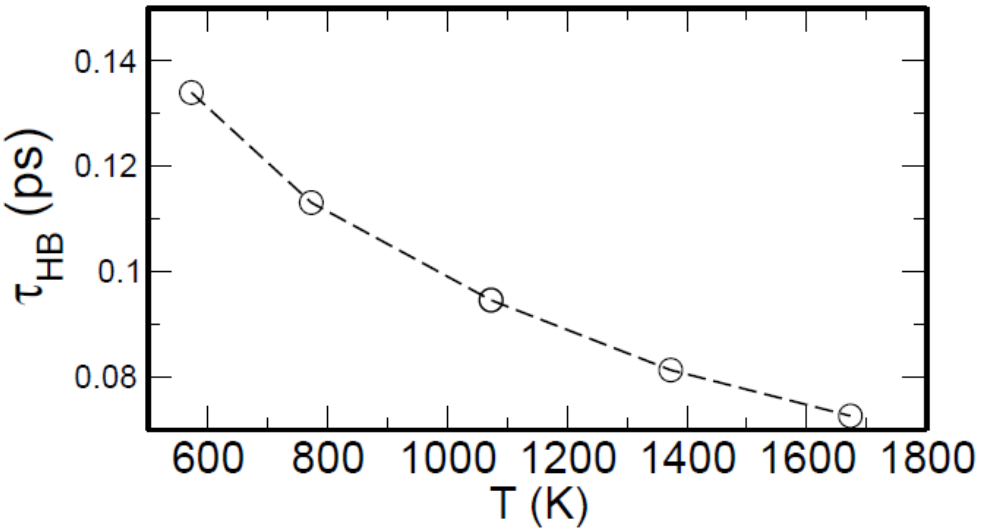
$$D = \frac{1}{6}\frac{d}{dt}\langle \Delta r(t)^2 \rangle$$

Deuterium diffusion in Sn metal liquid

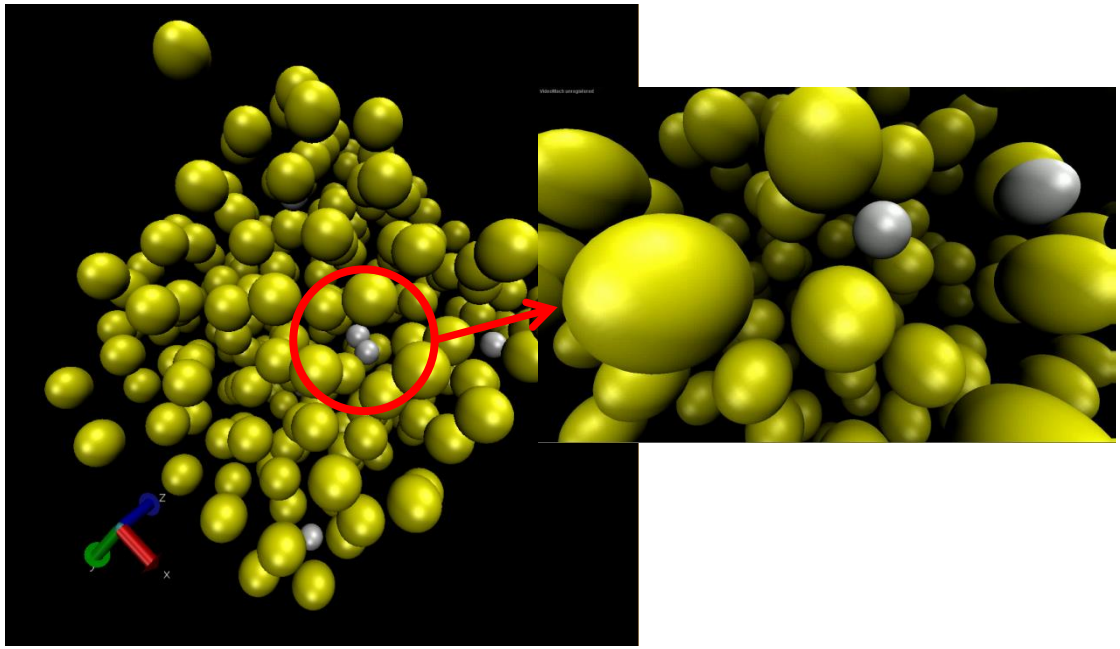




~2ps, 10^5 MD steps

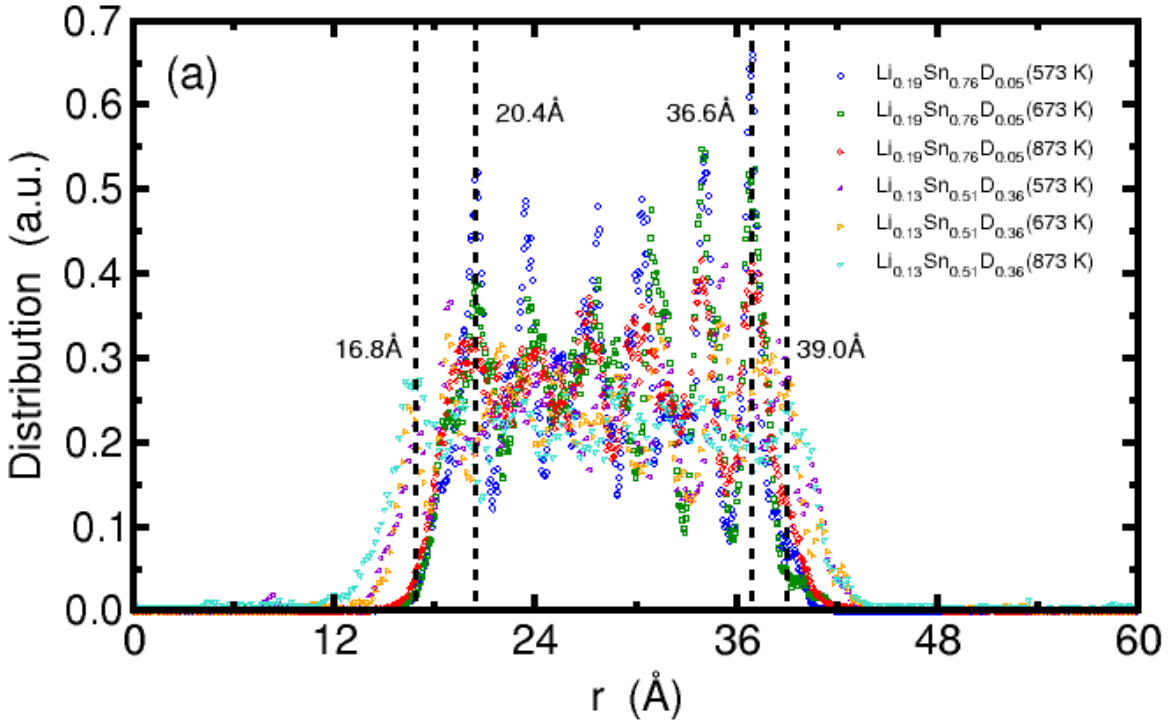


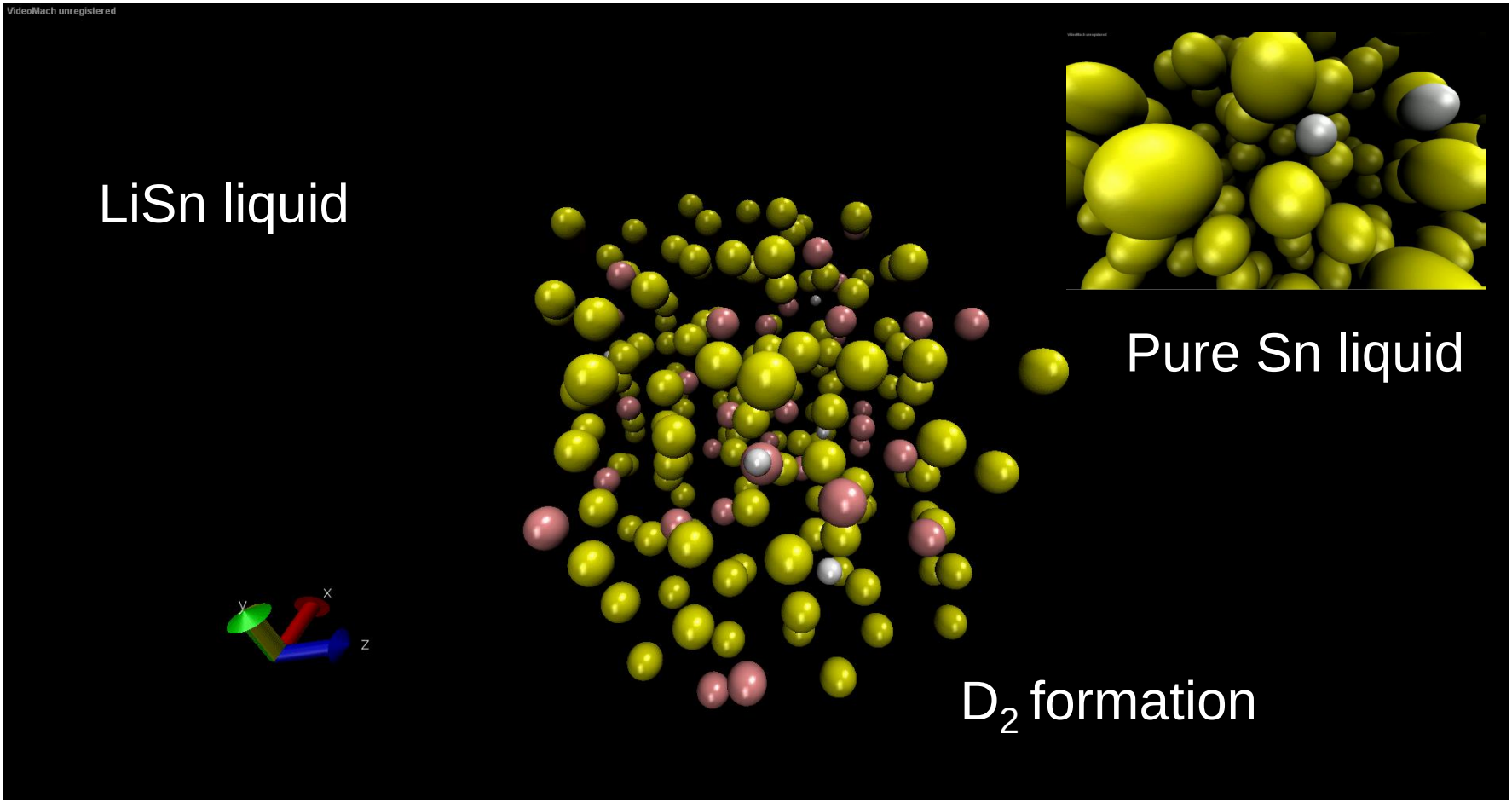
1. D does not form bonds with Sn;
2. D does not form bonds with other D;
3. Good for D distraction.



LiSnD liquid slab

1、ABACUS: LCAO-DZP
2、BOMD-NVT;
4、Time step: 0.2 fs, total time: 20 ps (100,000 steps);
5、Li : Sn = 1:4, T=573 K,673 K and 873 K ,
deuterium for 10 and 100.

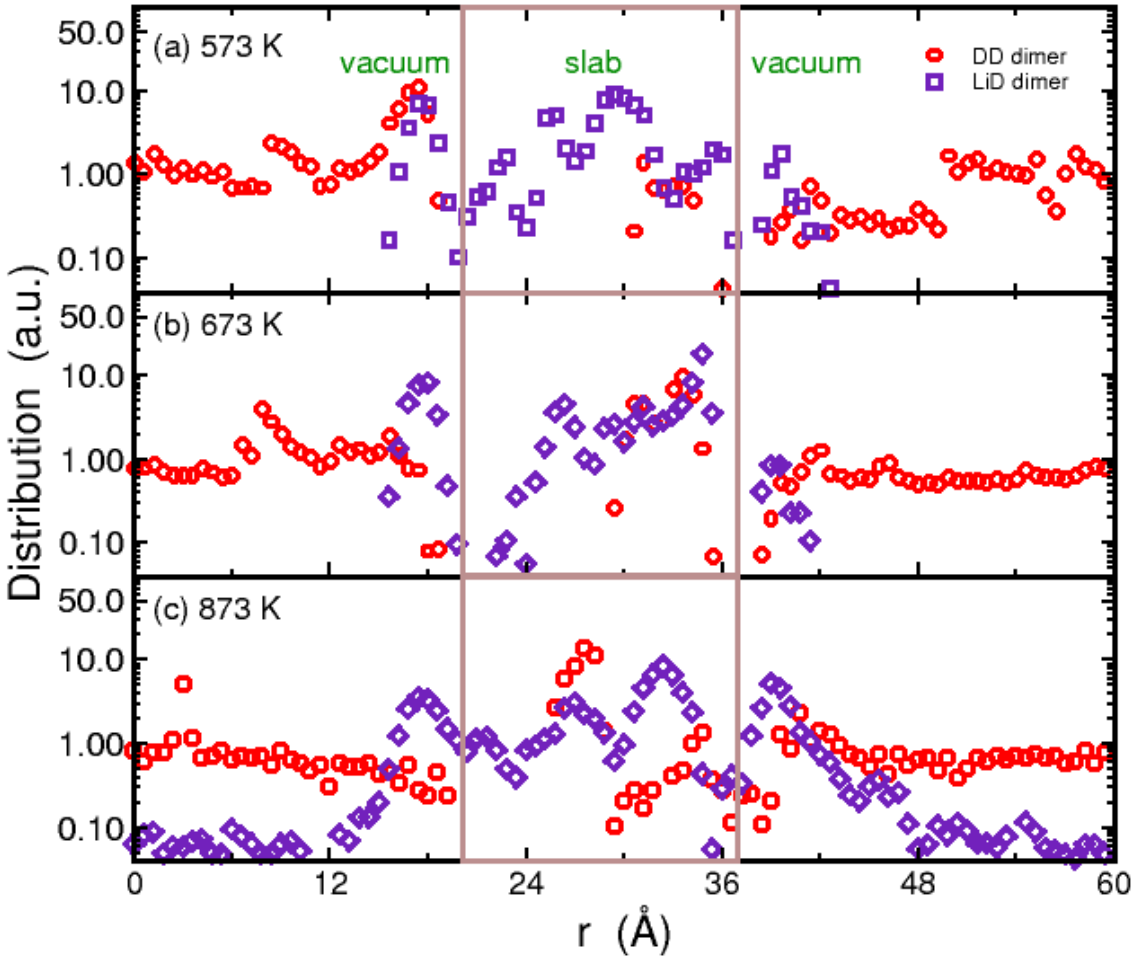



VideoMach unregistered
LiSn liquid
Pure Sn liquid
X
Y
Z
D_2 formation

(a) At 573 K and 673 K, D_2 dimer may escape to the vacuum.

(a) At 873 K, small mount of LiD dimer may also escape to vacuum.

In prepartion



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育天下英才

中國科學技術大學
建校三十周年誌慶

嚴濟慈 題

一九八八年五月