VASP - Best Practices Workshop

Weine Olovsson National Supercomputer Centre (NSC), Linköping University NAISS-ENCCS training, online 4-5th Apr 2023



VASP - Best Practices Workshop





https://www.nsc.liu.se/

https://www.naiss.se/

NAISS



https://enccs.se/

NSC is part of:

- LINKÖPING UNIVERSITY liu.se

NSC partners: <u>SAAB</u>, <u>SMHI</u>, <u>MET Norway</u>



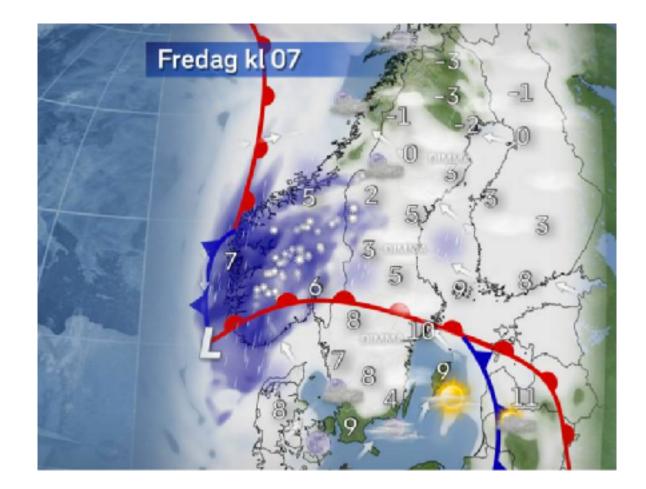


National Supercomputer Centre (NSC)

NAISS <u>National Academic Infrastructure for Supercomputing in Sweden</u>







Tetralith (2018 -) 1908 x 2 x 16 cores, Intel Xeon Gold 6130 NAISS

Sigma (2018 -) 110 x 2 x 16 cores, Intel Xeon Gold 6130 I.U



Knut and Alice Wallenberg Foundation

NSC academic clusters

- <u>Top500</u> no. 209 (74)

BerzeLiUs (2021 -) Nvidia DGX SuperPOD, 60 x 8 A100 GPUs - to be increased with 34 nodes in 2023 <u>Top500</u> no. 110 (82)



- PhD in Physics 2005 @Uppsala Univ.
- PostDoc @Kyoto Univ. 4y, @Leoben Univ. 1y
- Application Expert @NSC, 2011 (50%), 2016 (90%)
- 10% theoretical spectroscopy @IFM, LiU
- Electronic structure calculations
- @NSC: VASP, QE, WIEN2k, GPAW, ...



National Supercomputer Centre in Linköping Sweden

About myself

Information / Schedule

Tuesday 4th April

- 10:00 -11:00 Introduction & Basic Theory 11:00 -12:00 VASP - Basics
- 12:00 -13:00 Lunch
- 13:00 -15:00 Hands-on session (guided)
- 15:00 -17:00 Hands-on session

Wednesday 5th April

- 10:00 -11:00 Running & Performance 11:00 -12:00 Cont., Utilities & Summary
- 12:00 -13:00 L u n c h
- 13:00 -15:00 Hands-on session (guided)
- 15:00 -17:00 Hands-on session

10-15 min breaks every hour

- https://www.nsc.liu.se/support/Events/VASP_workshop_2023/
- <u>https://enccs.se/events/vasp-best-practices-workshop/</u>



- Weine Olovsson organizer & presentations
- Thor Wikfeldt (ENCCS) organizer & helper
- Qiang Li (ENCCS) helper
- Diana lusan (UPPMAX) helper
- Pavlin Mitev (UPPMAX) helper
- Luis Casillas Trujillo (NSC) helper
- <u>support@nsc.liu.se</u> Tetralith accounts

Workshop organization

- Basic theory (PAW)
- General considerations
- Focus on practical aspects of running VASP
- Benchmarks, examples
- Common problems

VASP - Best Practices Workshop

... at specific supercomputer centres

• Influential parameters, NPAR/NCORE, ALGO, NSIM, KPAR, ...

... clickable links are <u>underlined</u>



Wiki and Manual **Check in detail!** • Examples, tutorials

Presentations

• Forum

- Also other resources, materials and tools for VASP (see presentation 4.)
- Peter Larsson's old blog at NSC: <u>https://www.nsc.liu.se/~pla/</u>
- NSC VASP installations: <u>https://www.nsc.liu.se/software/installed/tetralith/vasp/</u>

Questions / trouble @NSC clusters? <u>support@nsc.liu.se</u>





Find all the links: https://vasp.at/

1. Introduction & Basic Theory

Weine Olovsson National Supercomputer Centre (NSC), Linköping University NAISS-ENCCS training, online 4-5th Apr 2023



VASP - Best Practices Workshop





https://www.nsc.liu.se/

https://www.naiss.se/

NAISS



https://enccs.se/

VASP: short background

- PAW-method
- DFT, **post-DFT** (HSE06, GW, ...)
- Born-Oppenheimer Molecular Dynamics
- widely used in Academia/Industry
 - Efforts from Intel & Nvidia for optimization
- 20-25% of Tetralith usage

... clickable links are <u>underlined</u>



Schrödinger Equation

Time-independent SE

 $H\Psi = E\Psi,$

solid ~10²³ particles...

Born-Oppenheimer approx. = 0 $H = T + T_n + V_{int} + V_{nn} + V_{ext} = -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 - \sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 + \frac{\hbar^2}{2M_I} \nabla_I^2$ $+\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}+\frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J \cdot e^2}{|\mathbf{R}_I-\mathbf{R}_J|}-\sum_{i=I}\frac{Z_I VI_I}{|\mathbf{r}_i-\mathbf{R}_J|},$

How to solve it?

"The general theory of quantum mechanics is now almost complete, ..."

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

"It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation"

Dirac, Proc. R. Soc. Lond. Ser. A **123**, 714 (1929)



Density Functional Theory (DFT)

Use electron probability density $n(\mathbf{r})$ instead of Ψ ...

(1) The potential V_{ext} of a system is determined uniquely, except for a constant by the ground state density $n(\mathbf{r})$

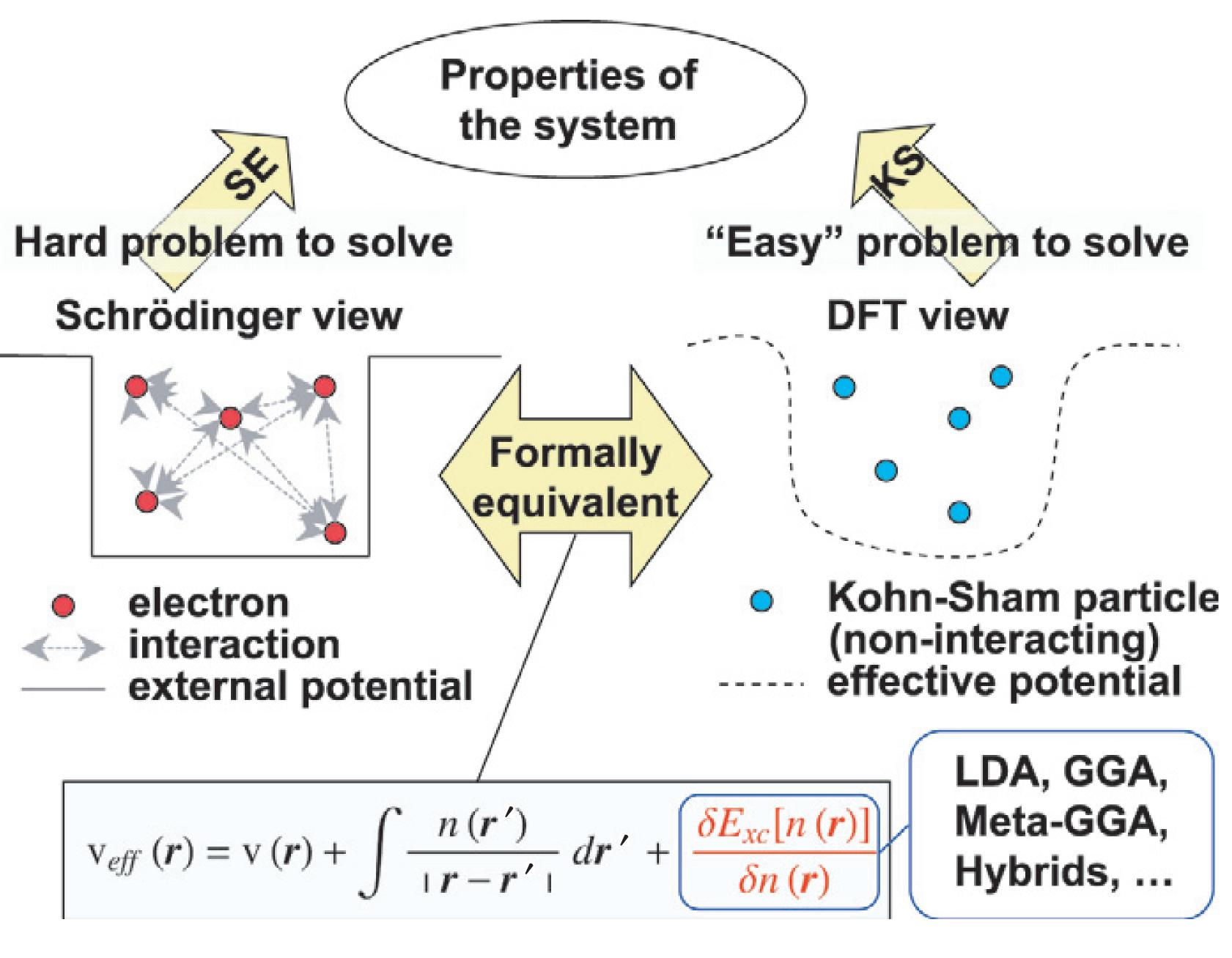
(2) The total energy functional E[n], for a given V_{ext}, assumes its minimal value for the correct electron density n(r) of the ground state

Ansatz: $E_{KS}[n] = \int d^3 r V_{ext}(\mathbf{r}) d^3 r V_{ext}(\mathbf{r})$

for independent electrons (mean field theory)

Hohenberg & Kohn, PRL **136**, B864 (1964) Kohn & Sham, PRL **140**, A1133 (1965)

$$n(\mathbf{r}) + T_s[n] + E_{xc}[n] + \int \int d^3r d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},$$



Mattsson et al., Modelling Simul. Mater. Sci. Eng. 13, R1 (2005)

Exchange-Correlation Functional

All difficulties now included in the XC-functional, need to find an approximation...

$$E_{xc}^{LDA}[n] = \int dr^3 n(\mathbf{r}) \boldsymbol{\varepsilon}_{xc}(n(\mathbf{r})),$$

$$E_{xc}^{GGA}[n] = \int d^3r n(\mathbf{r}) \boldsymbol{\varepsilon}_{xc}(n(\mathbf{r}), |\nabla n|),$$

GGA: PBE, AM05, PBEsol, ... meta-GGA: SCAN, ... mixing with exact-X: HSE06, ...

many choices, commonly used are e.g. PBE, HSE06, ...

Local Density Approximation (LDA) homogeneous electron gas

Generalized Gradient Approximation (GGA)



Using periodicity

The Bloch theorem states that the one-electron wavefunctions obey the equation:

$$\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = \psi_{n\mathbf{k}}(\mathbf{r})e^{i}$$

where \mathbf{R} is any translational vector leaving the Hamiltonian invariant.

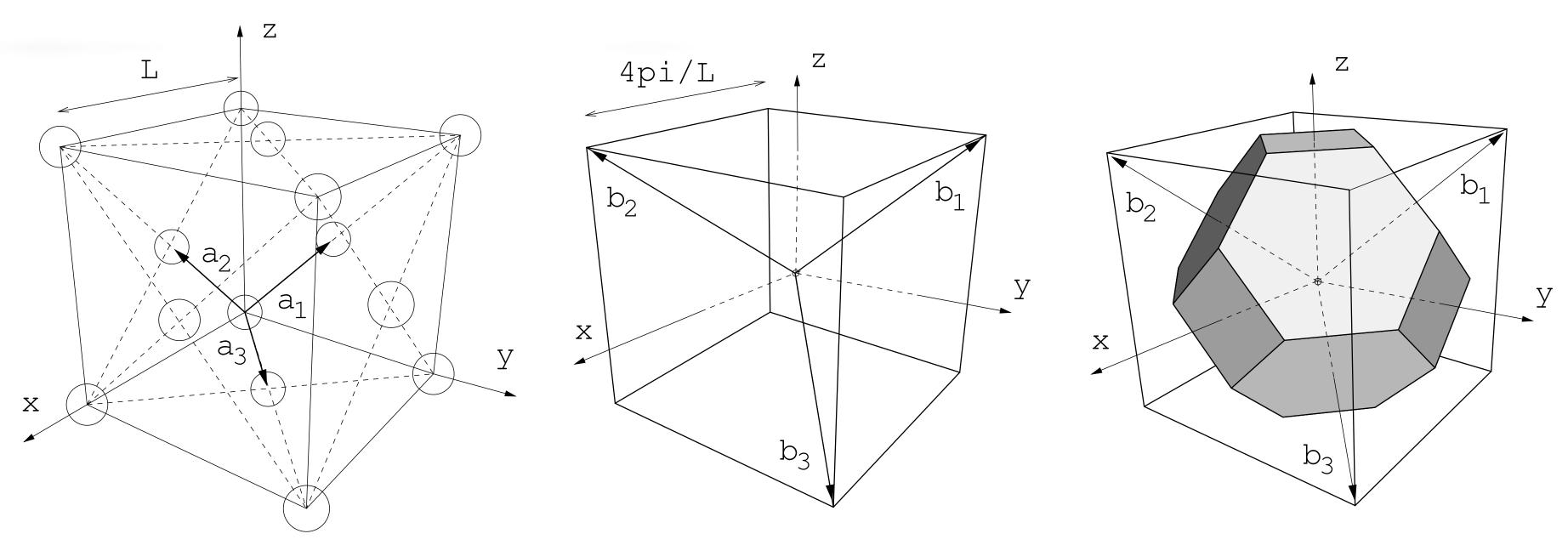
k is usually constrained to lie within the first Brillouin zone in reciprocal space.

> The intractable task of determining $\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)$ (for $N \sim 10^{23}$) has been reduced to calculating $\psi_{n\mathbf{k}}(\mathbf{r})$ at a discrete set of points $\{\mathbf{k}\}$ in the first BZ, for a number of bands that is of the order of the number of electrons per unit cell.

from Marsman: <u>https://www.vasp.at/mmars/day1.pdf</u>

 \mathbf{kR}

Using periodicity



А

 $\mathbf{b}_1 = rac{2\pi}{\Omega} \mathbf{a}_2 imes \mathbf{a}_3 \quad \mathbf{b}_2 =$

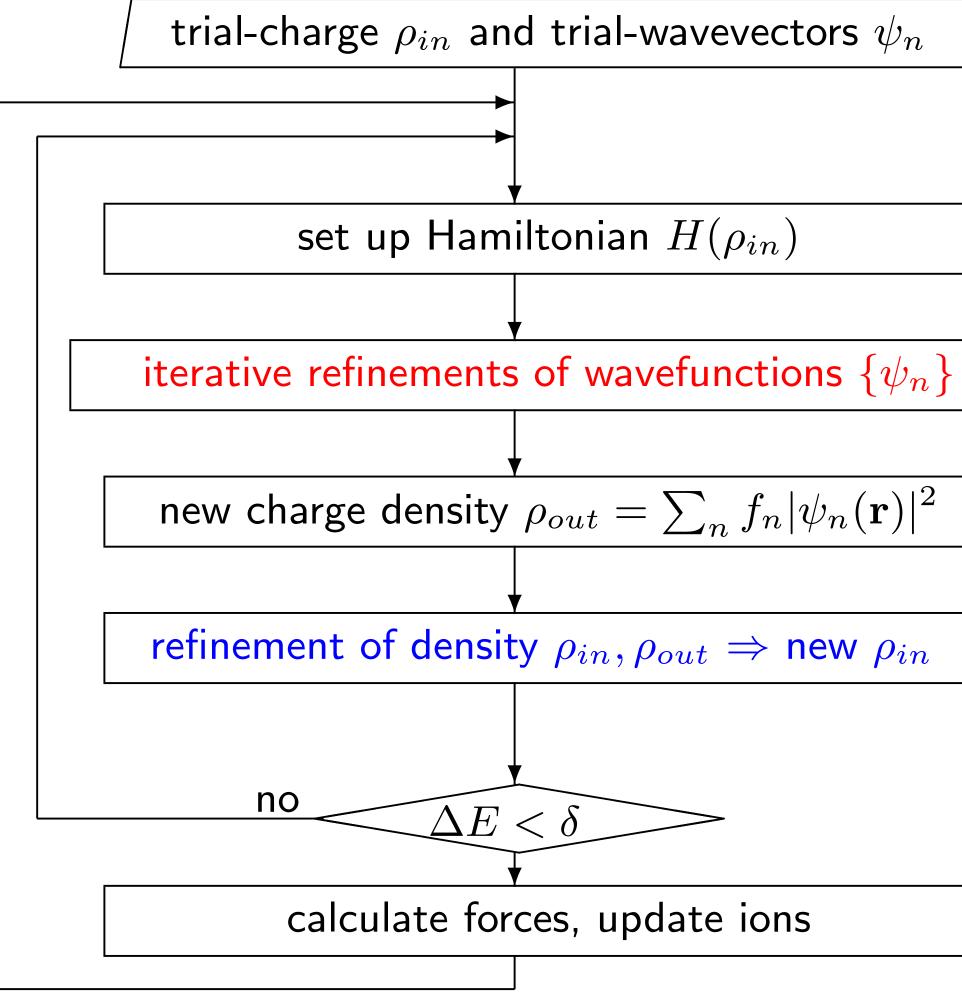
 $\Omega = \mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 \qquad \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}$

from Marsman: https://www.vasp.at/mmars/day1.pdf



$$=\frac{2\pi}{\Omega}\mathbf{a}_3\times\mathbf{a}_1\quad\mathbf{b}_3=\frac{2\pi}{\Omega}\mathbf{a}_1\times\mathbf{a}_2$$

Self-consistent iterations



from Marsman: <u>https://www.vasp.at/mmars/day1.pdf</u>

$$b_{ut} = \sum_{n} f_n |\psi_n(\mathbf{r})|^2$$

$$\rho_{in}, \rho_{out} \Rightarrow \mathsf{new} \ \rho_{in}$$

- two subproblems optimization of $\{\psi_n\}$ and ρ_{in}
- refinement of density: DIIS algorithm P. Pulay, Chem. Phys. Lett. 73, 393 (1980)
- refinement of wavefunctions: DIIS or Davidson algorithm

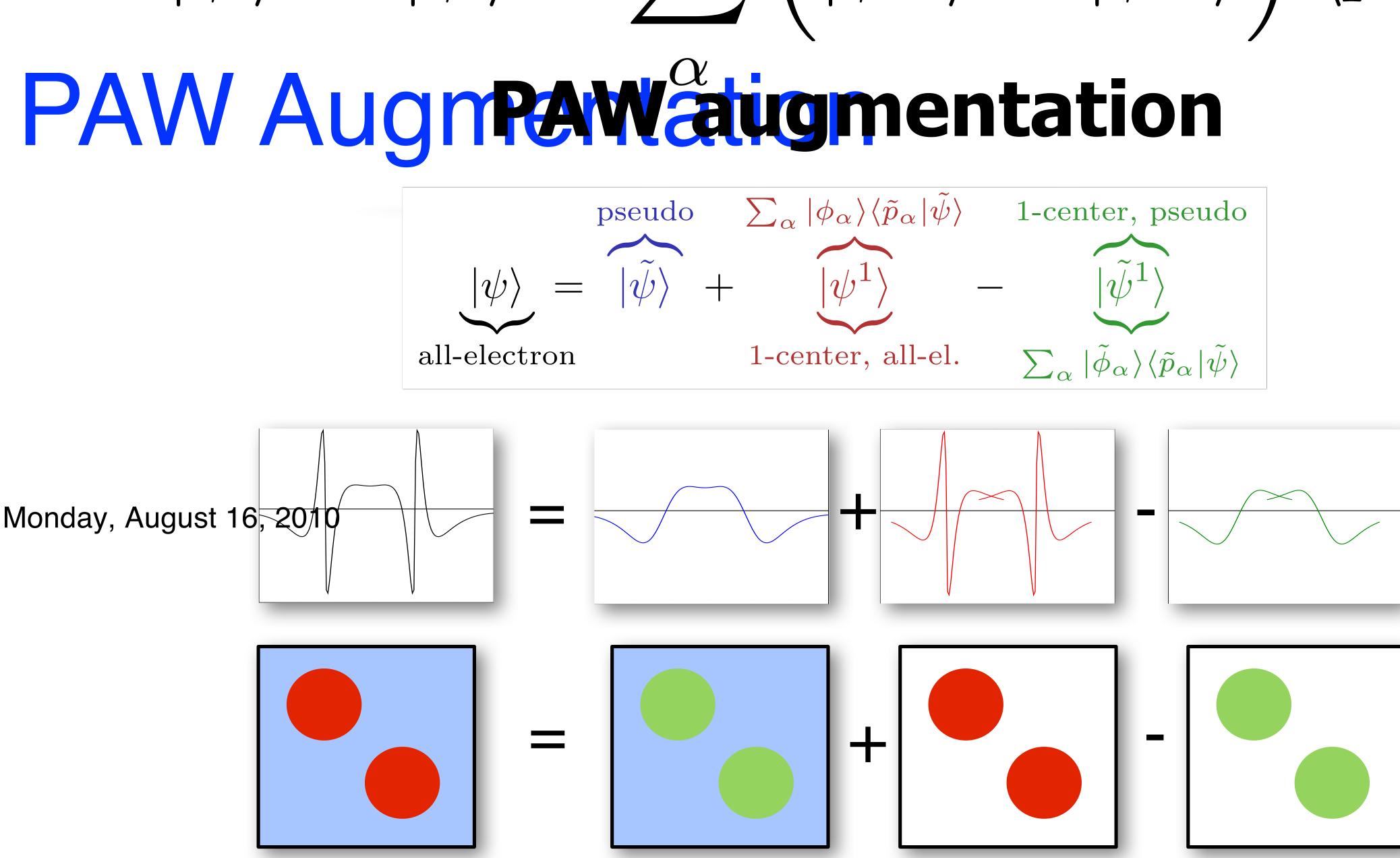
Why PAW?

- Goal: both accurate (LAPW) and fast (e.g. USPP) method
- Want to keep all-electron (AE) wave function
- Focus on valence electrons (frozen core) chemical bonding
- Fast calculation in *reciprocal space* using FFT (plane waves)
- Solution: Projector Augmented Wave (PAW) method

Plane waves & Augmentation

- Rapid wave oscillations close to nucleus
- need too many plane waves!
 Strongly localised states at atoms
- Split into *interstitial* and *augmentation* (sphere) regions smooth pw
- No overlap between spheres (one-centre expansion)
- PAW: Energy and potential independent wave functions

therefore ->

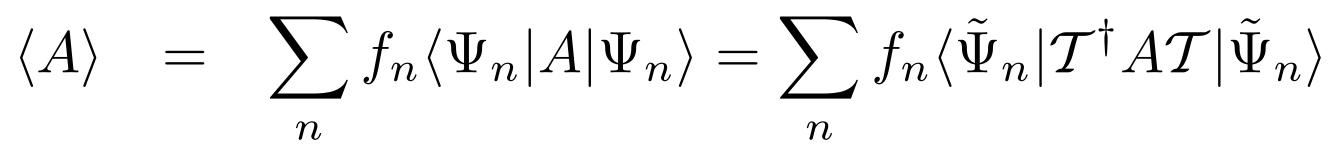


from Blöchl: http://www2.pt.tu-clausthal.de/atp/downloads/lyngby2_paw.pdf Monday, August 16, 2010

Transformation theory

True AE wave function and *auxiliary* PS wf related via transformation operator:

$$|\Psi_n
angle = \mathcal{T}|\tilde{\Psi}_n
angle$$



Expectation values can be evaluated for *true* AE or *auxiliary* PS waves

Blöchl et al. https://arxiv.org/abs/cond-mat/0201015v2



Kohn-Sham equation:

$$H|\Psi_n\rangle = |\Psi_n\rangle\epsilon_n$$

Can write Schrödinger-like equation:

$$\mathcal{T}^{\dagger} H \mathcal{T} | \tilde{\Psi}_n \rangle = \mathcal{T}^{\dagger} \mathcal{T} | \tilde{\Psi}_n \rangle \epsilon_n$$

Transformation operator

$$\mathcal{T} = 1 + \sum_{R} \mathcal{S}_{R}$$

FO unity in *interstitial*, outside

augmentation sphere R

B

Inside sphere R, describe by **AE partial waves**, undetermined coefficients *c*_i

$$\Psi(\mathbf{r}) = \sum_{i \in R} \phi_i(\mathbf{r}) c_i \quad \text{for} \quad |\mathbf{r} - \mathbf{R}_R| < r_{c,R}$$

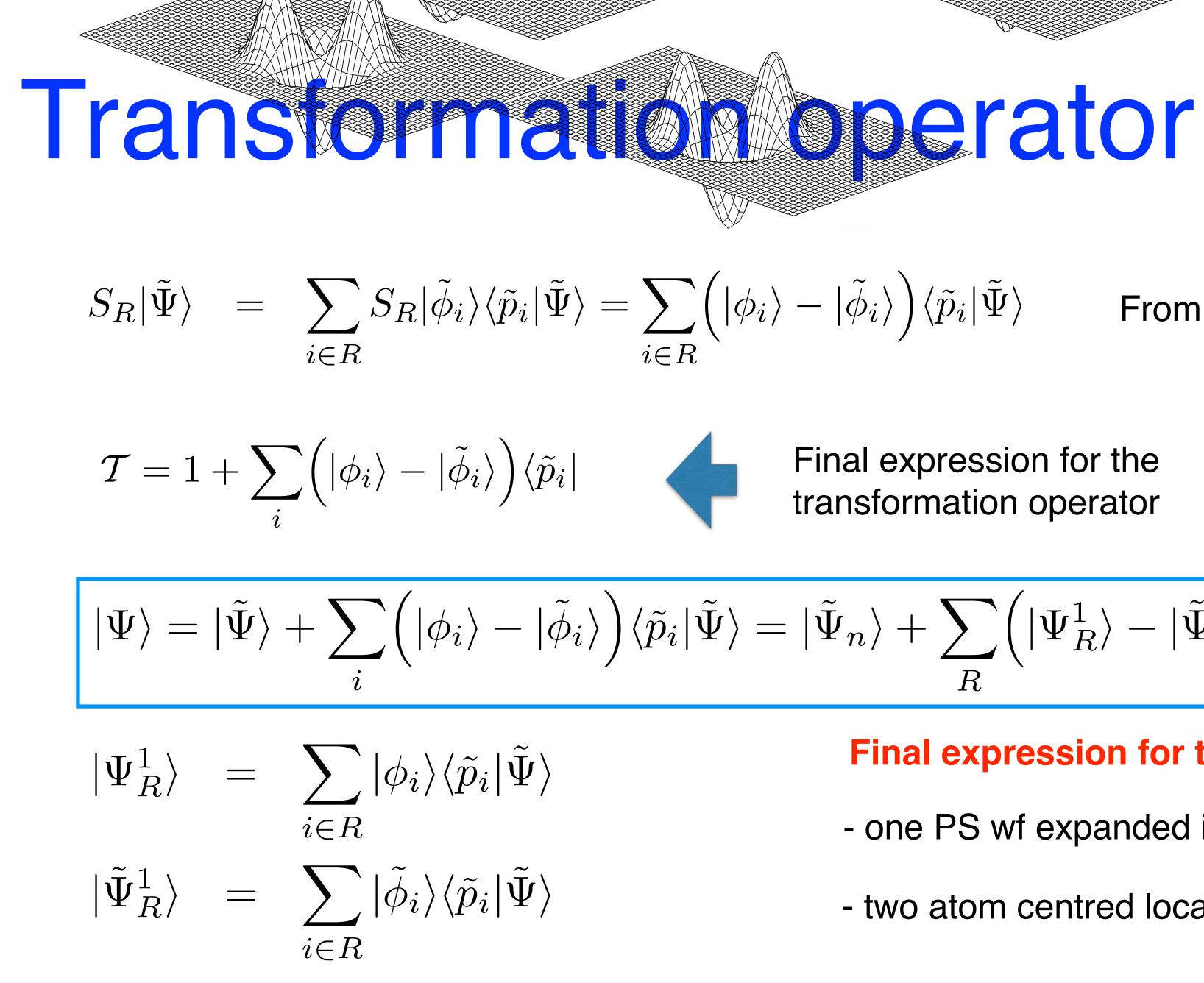
Relate AE partial wave with **PS partial wave**, through *local* transformation operator S

 $< r_{c,R}$ Expand PS wf in PS partial waves

ion

nt for above to hold

<u>1015v2</u>



Blöchl et al. https://arxiv.org/abs/cond-mat/0201015v2

- From using the previous relations

$$\langle u_n \rangle + \sum_R \left(|\Psi_R^1 \rangle - |\tilde{\Psi}_R^1 \rangle \right)$$

Final expression for the *true* AE wf:

- one PS wf expanded in plane waves
- two atom centred localised functions

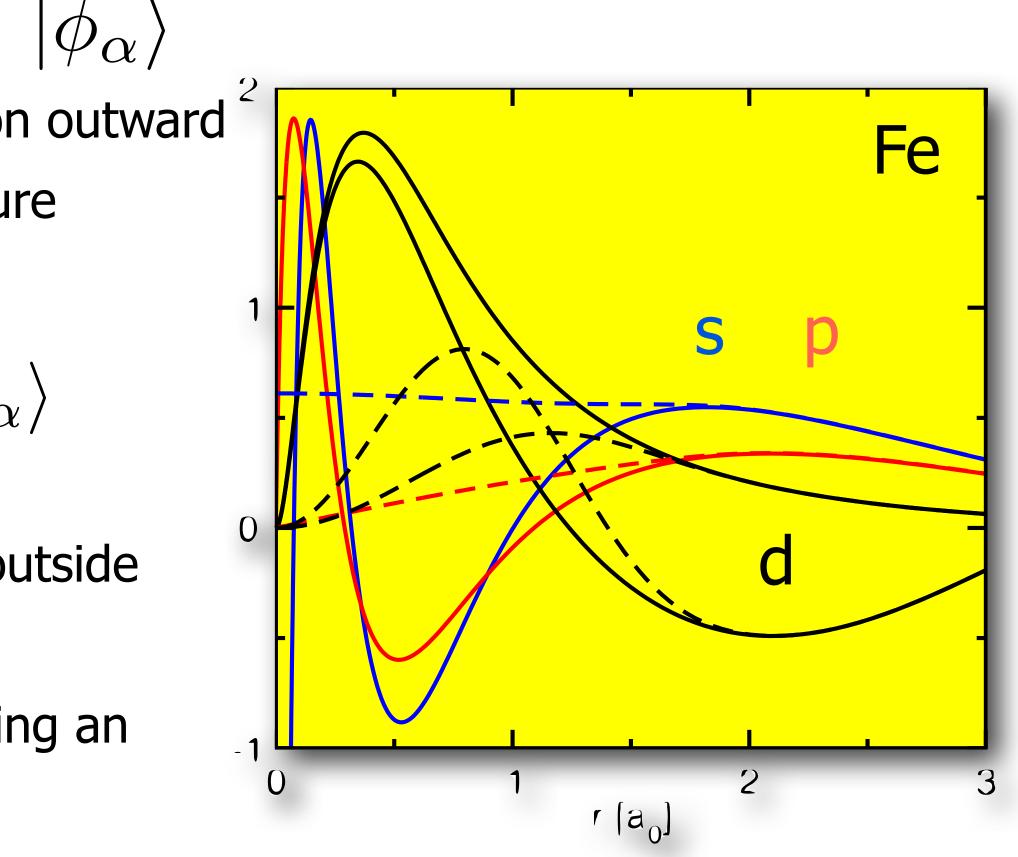
Partial waves

- all-electron partial waves $|\phi_{\alpha}\rangle$
 - integrate Schrödinger equation outward
 - have the correct nodal structure
- pseudo partial waves $|\phi_{\alpha}\rangle$



- smooth inside
- identical to ae partial waves outside
- n-n_{core} nodes
- usually constructed by adjusting an dependent potential

from Blöchl: http://www2.pt.tu-clausthal.de/atp/downloads/lyngby2_paw.pdf



Projector functions

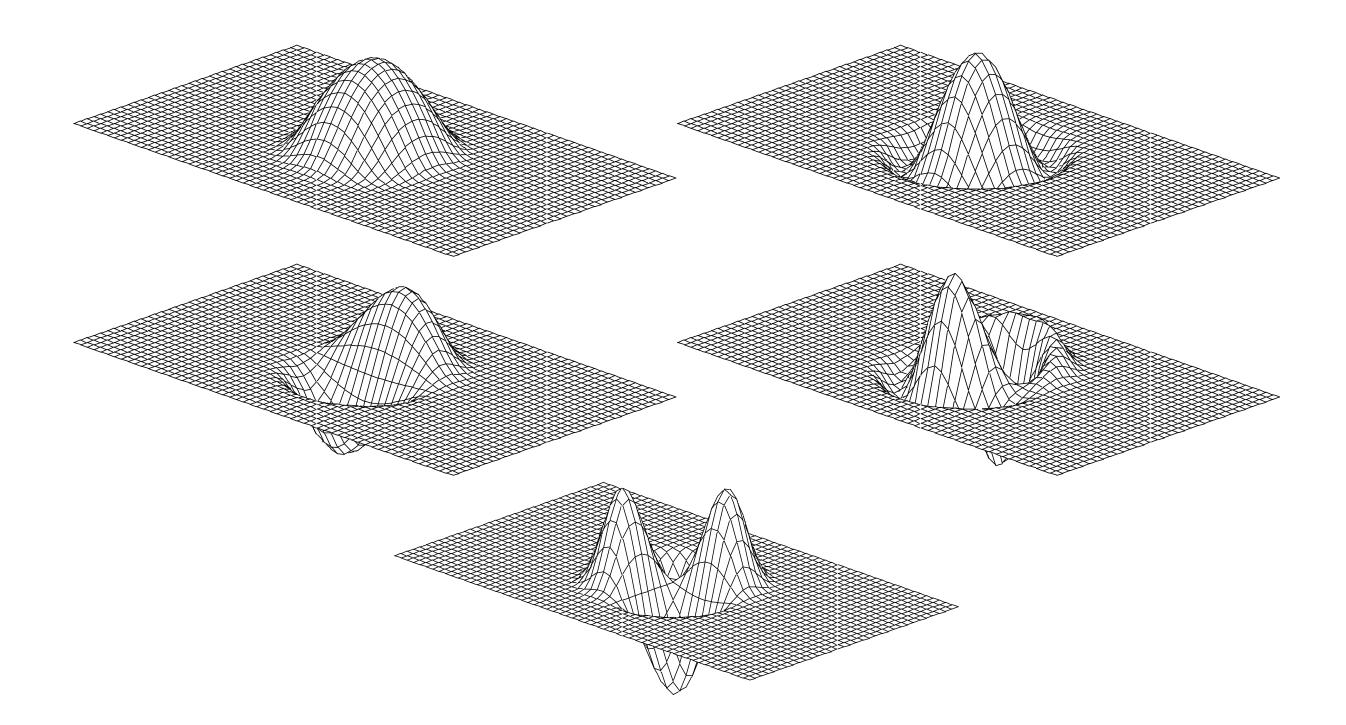


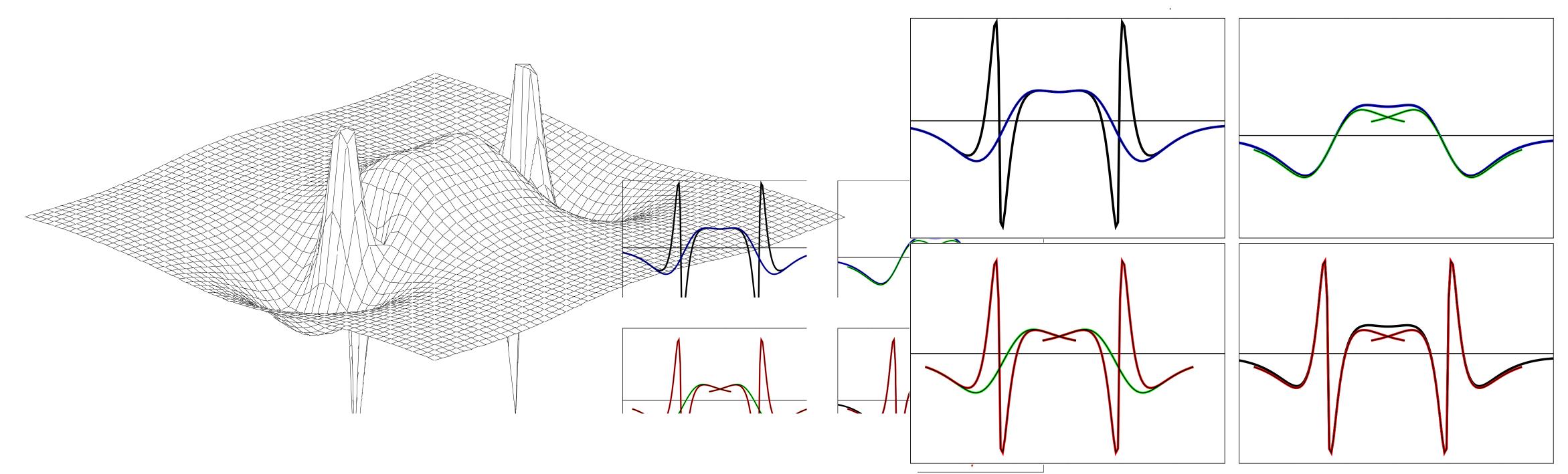
Figure 1: Top: projector functions of the Cl atom for two s-type partial waves, middle: p-type, bottom: d-type.

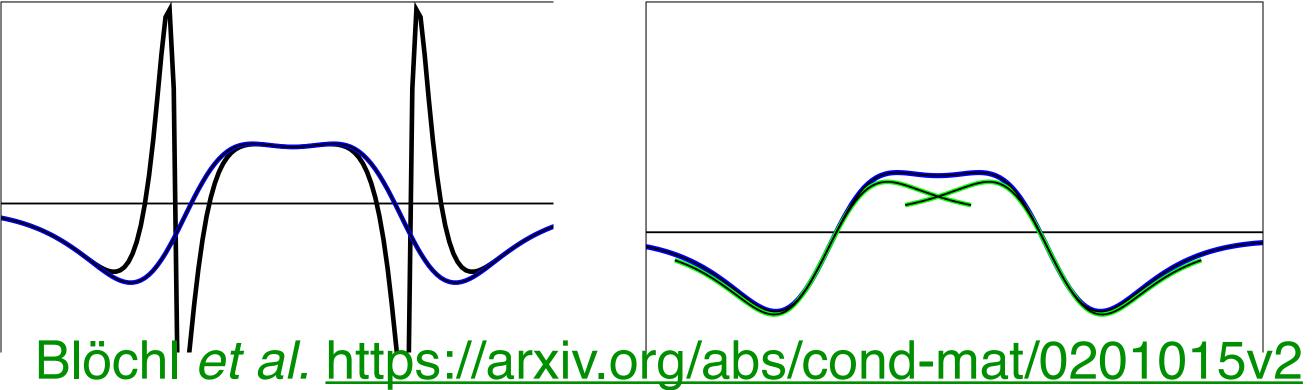
Blöchl et al. https://arxiv.org/abs/cond-mat/0201015v2

- Localised
- Angular momentum of partial waves



Wave functions



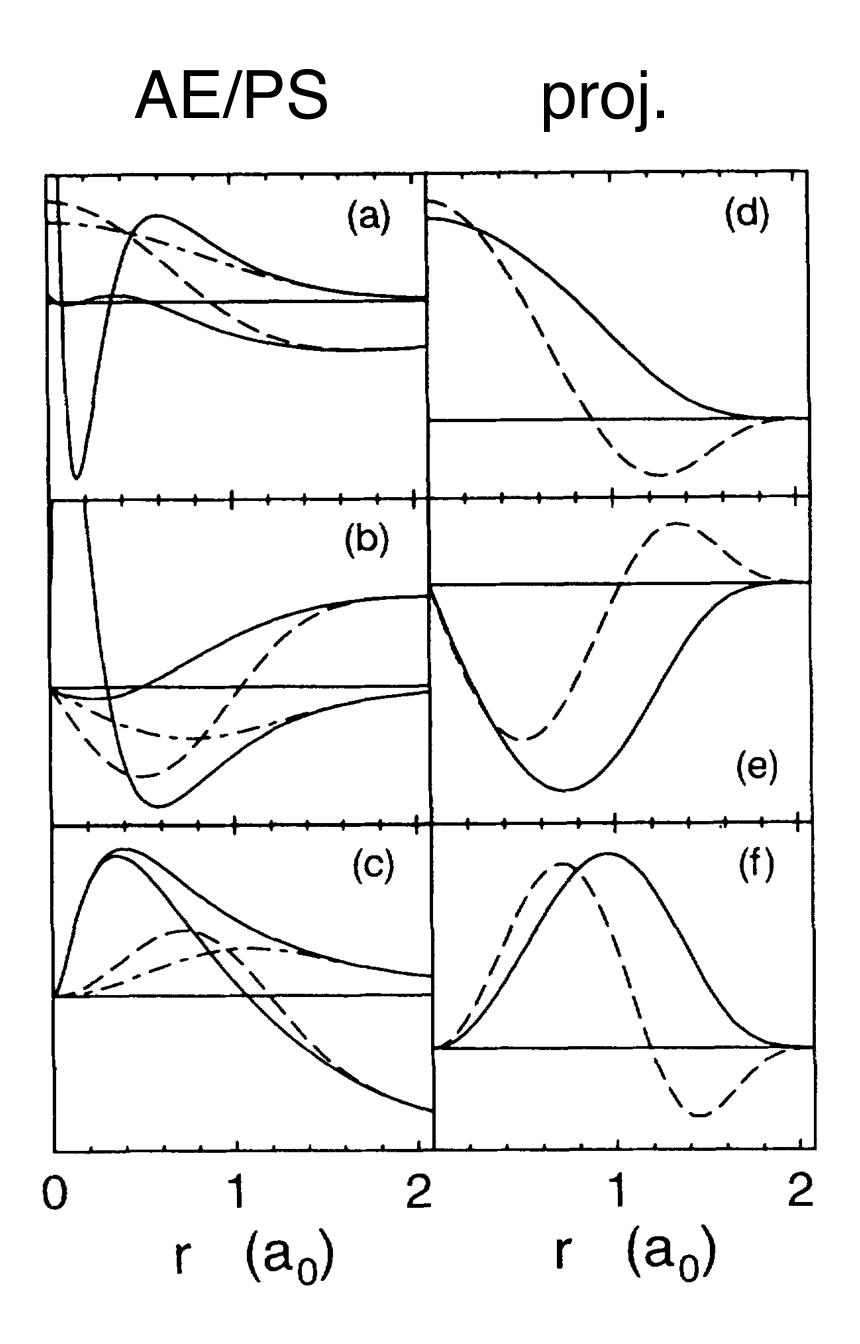


ile and its decomposition of the the two one-center expansions. >-right: auxiliary wave function ne two partial wave expansions; l wave expansion.

More examples

FIG. 1. Partial waves and projectors for Mn. Left panel: AE partial waves (solid lines) and PS partial waves (dashed and dash-dotted lines). The "first" PS partial wave is a dash-dotted line. Right panel: first (solid line) and second (dashed line) projector functions. (a) and (d) show the results for the first and the second partial wave of the *s* angular momentum channel, respectively, (b) and (e) for the *p* channel, and (c) and (f) for the *d* channel. 3s and 3p functions are treated as valence states. Functions are scaled individually.

Blöchl PRB 50, 17953 (1994)



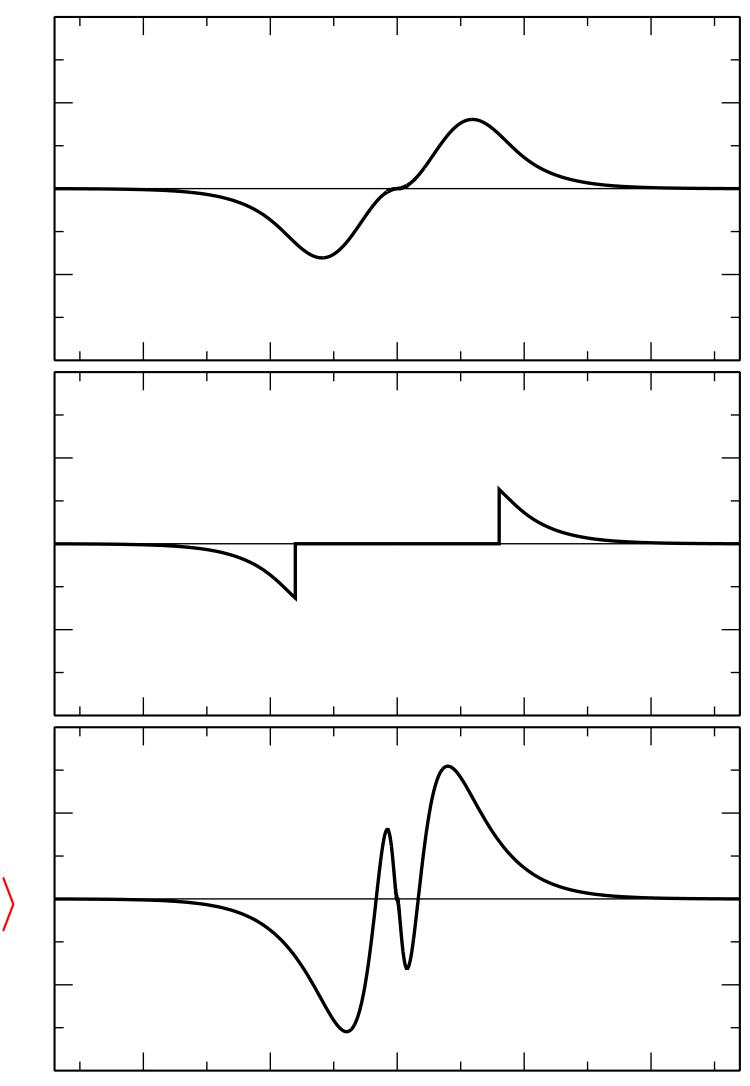
PAW Augmentation

$|\widetilde{\psi}_n angle$

$|\widetilde{\psi}_n\rangle - \sum_i |\widetilde{\phi}_i\rangle \langle \widetilde{p}_i |\widetilde{\psi}_n\rangle$

 $|\tilde{\psi}_n\rangle - \sum_i |\tilde{\phi}_i\rangle\langle \tilde{p}_i|\tilde{\psi}_n\rangle + \sum_i |\phi_i\rangle\langle \tilde{p}_i|\tilde{\psi}_n\rangle$

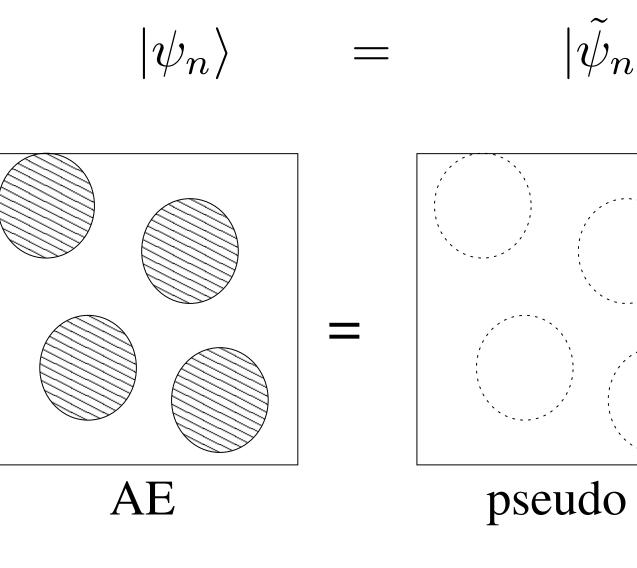
from Marsman: <u>https://www.vasp.at/mmars/day1.pdf</u>





PAW Augmentation

• Character of wavefunction: $c_{lm\epsilon} = \langle \tilde{p}_{lm\epsilon} | \tilde{\psi}_n \rangle$



Same trick works for

- Wavefunctions
- Charge density

from Marsman: <u>https://www.vasp.at/mmars/day1.pdf</u>

 $|\tilde{\psi}_n\rangle = -\sum |\tilde{\phi}_{lm\epsilon}\rangle c_{lm\epsilon} + \sum |\phi_{lm\epsilon}\rangle c_{lm\epsilon}$ +pseudo-onsite AE-onsite

- Kinetic energy
- Exchange correlation energy
- Hartree energy

Iotal Energy

$$\begin{split} \tilde{E} &= \sum_{n} f_{n} \langle \tilde{\psi}_{n} | -\frac{1}{2} \Delta | \tilde{\psi}_{n} \rangle + E_{xc} [\tilde{\rho} + \rho] \\ \mathsf{PW} \text{ grid} & E_{H} [\tilde{\rho} + \hat{\rho}] + \int v_{H} [\tilde{\rho}_{Zc}] (\tilde{\rho}(\mathbf{r}) + \rho] \\ \tilde{E}^{1} &= \sum_{\text{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \tilde{\phi}_{i} | -\frac{1}{2} \Delta | \tilde{\phi}_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{\tilde{E}^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{local}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\} \\ \frac{E^{1}}{\mathrm{radial grid}} &= \sum_{\mathrm{sites}} \left\{ \sum_{(i,j)} \rho_{ij} \langle \phi_{i} | -\frac{1}{2} \Delta | \phi_{j} \rangle + \overline{E_{xc}} \right\}$$

from Marsman: <u>https://www.vasp.at/mmars/day1.pdf</u>

$$E = \tilde{E} + E^1 - \tilde{E}^1$$
 three terms

 $\hat{\rho} + \tilde{\rho}_c] +$

 $\hat{\rho}(\mathbf{r})) d^3\mathbf{r} + U(\mathbf{R}, Z_{\text{ion}})$ $\frac{1}{2c}[\tilde{\rho}^1 + \hat{\rho} + \tilde{\rho}_c] +$ $) + \hat{\rho}(\mathbf{r}) d^3 \mathbf{r} \bigg\}$ $\frac{1}{2c[\rho^1 + \rho_c]} + \frac{1}{2c[\rho^1 + \rho_c]}$

What are the approximations?

- Frozen core
- Plane wave expansion, energy
- Partial wave expansion (1-2 per angular momentum)

can be relaxed: Marsman & Kresse, JCP 125, 104101 (2006)

y cut-off
$$\frac{1}{2}|\mathbf{G} + \mathbf{k}|^2 < E_{\text{cutoff}}$$

PAW: Things to note

- All-electron method (valence states orthogonal to core)
- Frozen core approximation
- Plane waves: FFT in reciprocal space, fast calculations
- Forces from total energy expression

• PAW point-of-view: LAPW special case, PP an approximation

Accuracy

Compare with FPLAPW method (WIEN2k):																	
н																	He
0.1																	0.0
Li	Be			A/D/	(14/)	_	В	с	Ň	0	F	Ne					
0.2	0.1				•••) _{(V.}	ASP) =	0.3	0.3	10.6	8.3	1.5	0.1					
Na	Mg						Al	Si	Р	S	CI	Ar					
0.0	0.7						0.3	2.0	3.8	3.3	4.0	0.1					
К	Ca	a Sc Ti V Cr Mn Fe Co Ni Cu Zn								Ga	Ge	As	Se	Br	Kr		
0.1	0.2	0.4 0.9 1.3 3.1 1.4 3.4 3.4 2.0 0.4 0.3								0.2	2.4	1.7	1.5	1.5	0.1		
Rb	Sr	Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd									In	Sn	Sb	Te	1	Xe	
0.1	0.1	1 0.5 2.7 7.3 5.5 8.3 2.3 5.4 4.4 4.1 1.4											0.2	0.1	0.5	0.9	0.1
Cs	Ва	Lu	Hf	Та	W	Re	Os	lr	Pt	Au	Hg	TI	Pb	Bi	Ро	At	Rn
0.3	0.7	4.3	1.2	1.0	3.5	4.3	3.8	1.9	2.5	5.9	0.5	0.4	0.6	0.4	0.4		0.0

Lejaeghere et al. Crit. Rev. Solid State Mat. Sci. 39, 1 (2014)

	AE AE								PAW								USPP						NCPP dels							
		Elk exciting	-aims/tight	FHL-aims/really_tig FHL-aims/tier2	FLEUR FPLO/default	FPLO/T+F	FPLO/T+F+S RSPt	WIEN2k/default	WIEN2k/enhanced WIEN2k/acc		GPAW06/GPAW	GPAW09/ABINIT	GPAW09/GPAW JTH01/ABINIT	JTH02/ABINIT	PSlib031/QE	PS1ib100/QE	VASP2007/VASP VASP2012/VASP	VASPGW2015/VASP	GBRV12/QE	GBRV14/CASTEP	1 1	OTFG9/CASTEP	SSSP/QE Vdb/CASTEP	Vdb2/DACAPO	TINIA/qq891HF	HGH/ABINIT HGH-NLCC/BigDFT	MBK2013/OpenMX	SP(PD0.1)/AB		ONCVPSP(SG15)2/CASTEF
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	exciting	0.3	0.5 0	0.5 0.1	0.5 3.9	1.0	0.9 0.8	3 1.7	1.8 0.2	2 0.8	3.8	1.3	1.5 1.	2 0.6	1.6	0.8 2	2.1 0.	.6 0.4	1.0	1.1 1	0 2.5	0.5 (0.3 6.4	6.3	13.4	2.2 1.3	L 2.1	0.7 1	l.4 1.3 1	1.4
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	RSPt				0.6 3.3		0.9	1.3		1.5	3.7	1.7	1.7 0.9				L.9 1.				.3 3.0).9 0.4			2.2 1.2		0.8 1	5 15	1.0
	WIEN2k/default	17 17	18 1	8 17	1.4 2.9		1.5 1.3		0.9 1.7	19	32	22	23 1	3 1 5	1.0	18 1		.8 1.8	1.2	1.9 1	9 38		.6 7.1		13.0	2.2 1.	7 1 9	16 2	2.1 2.1 2	21
		1.8 1.8	1.8 1	L.8 1.8	1.5 2.5		1.5 1.3				2.6	2.1	2.2 1.	1 1.5	1.6	1.8 1	L.4 1.		2.0	2.0 2	0 3.8		.7 6.9		12.3	2.8 1.6	5 1.5	1.7 1	L.9 1.9 1	
		0.3 0.2										1.3	1.5 1.	2 0.5	1.6	0.8 2													L.4 1.3 1	
														_	-		_				_					_			L.8 1.7 1	
	GPAW06/GPAW	3.8 3.8																											8.7 3.8 3	
	GPAW09/ABINIT	1.3 1.3	1.3 1	L.3 1.3	1.3 4.1	1.7	1.7 1.	5 2.2	2.1 1.3	3 1.5	3.6	(0.6 1.	5 1.4	2.0	1.5 2	2.4 1.	.4 1.3	1.6	1.6 1	6 2.5	1.4 1	.3 6.5	6.1	13.6	2.3 1.7	7 2.3	1.2 1	L.7 1.7 1	1.7
	GPAW09/GPAW	1.5 1.5	1.6 1	L.6 1.5	1.5 4.1	1.9	1.8 1.	7 2.3	2.2 1.5	5 1.6	3.5	0.6	1.	6 1.5	2.1	1.6 2	2.5 1.	.6 1.5	1.7	1.7 1	7 2.7	1.5 1	.4 6.5	6.1	13.6	2.5 1.8	3 2.3	1.5 1	L.8 1.8 1	1.8
>	JTH01/ABINIT	1.2 1.2	1.3 1	L.3 1.2	1.0 3.4	1.0	1.2 0.9	9 1.3	1.1 1.2	2 1.5	3.2	1.5	1.6	0.9	1.5	1.4 1	L.9 1.	4 1.3	1.5	1.5 1	5 3.0	1.4 1	.1 6.5	6.5	13.0	2.2 1.3	3 1.5	1.2 1	l. 4 1.4 1	1.4
N N	JTH02/ABINIT	0.6 0.6	0.7 0).7 0.6	0.6 3.6	0.9	0.9 0.	7 1.5	1.5 0.5	5 1.1	3.5	1.4	1.5 0.9	9	1.4	0.9 1	L.9 0.	.7 0.7	1.2	1.2 1	2 2.6	0.7 0	0.6 6.3	6.2	13.4	2.2 1.2	2 1.9	0.7 1	L.4 1.4 1	1.4
PZ	PSlib031/QE	1.6 1.6	1.7 1	l.7 1.6	1.5 3.3	1.5	1.4 1.0	5 1.8	1.6 1.6	5 2.0	3.0	2.0	2.1 1.	5 1.4		1.6 1	L.5 1.	.6 1.6	2.0	1.9 2	0 3.1	1.6	.5 6.1	5.8	12.8	2.4 1.6	5 1.7	1.5 2	2.1 2.2 2	2.1
	PSlib100/QE	0.9 0.8	1.0 1	L.O 0.8	0.8 3.9	1.3	1.3 1.3	1 1.8	1.8 0.8	3 1.1	3.8	1.5	1.6 1.4	4 0.9	1.6	1	L.7 1.	.0 0.8	1.1	1.2 1	2 2.2	0.9 0	0.7 6.1	5.9	13.5	2.1 1.4	1.9	0.9 1	L.6 1.6 1	1.6
	VASP2007/VASP	2.1 2.1	2.2 2	2.2 2.0	1.9 2.8	1.9	1.9 1.9	9 1.7	1.4 2.0	2.3	2.8	2.4	2.5 1.9	9 1.9	1.5	1.7	1.	.8 2.1	2.1	2.2 2	1 3.5	2.1	.9 6.5	6.1	12.4	3.0 2.2	2 1.7	1.9 2	2.5 2.4 2	2.5
	VASP2012/VASP	0.7 0.6	0.8 0).8 0.6	0.7 3.9	1.2	1.2 1.0	0 1.8	1.9 0.7	1.0	3.7	1.4	1.6 1.4	4 0.7	1.6	1.0 1	L.8	0.7	1.1	1.2 1	1 2.5	0.8	.6 6.5	6.3	13.4	2.2 1.2	2 2.1	0.9 1	L.6 1.5 1	1.6
	VASPGW2015/VASP	0.4 0.4	0.6 0	0.6 0.4	0.6 4.0	1.0	1.0 0.8	3 1.8	2.0 0.3	8 0.9	3.8	1.3	1.5 1.	3 0.7	1.6	0.8 2	2.1 0.	.7	1.1	1.1 1	1 2.6	0.5	.4 6.6	6.2	13.7	2.2 1.3	L 2.2	0.7 1	L.5 1.4 1	1.5
	GBRV12/QE	1.1 1.0	1.1 1	l.1 0.9	1.0 4.0	1.3	1.4 1.2	2 1.9	2.0 0.9	0.7	4.0	1.6	1.7 1.	5 1.2	2.0	1.1 2	2.1 1.	.1 1.1		0.4 0	1 2.6	1.0 0).8 6.3	6.4	15.3	2.3 1.4	1 2.1	1.2 1	L.6 1.5 1	1.6
	GBRV14/CASTEP	1.1 1.1	1.2 1	l.2 1.0	1.0 4.0	1.3	1.4 1.3	3 1.9	2.0 1.0	0.8	3.8	1.6	1.7 1.	5 1.2	1.9	1.2 2	2.2 1.	.2 1.1	0.4	С	3 2.6	0.9 0).9 6.2	6.3	15.0	2.4 1.6	5 2.1	1.1 1	l.5 1.5 1	1.5
<u>م</u>	GBRV14/QE	1.0 1.0	1.1 1	l.1 0.9	1.0 4.1	1.3	1.4 1.3	3 1.9	2.0 1.0	0.7	4.0	1.6	1.7 1.	5 1.2	2.0	1.2 2	2.1 1.	.1 1.1	0.1	0.3	2.6	1.0 0	0.8 6.3	6.3	15.2	2.3 1.4	2.1	1.2 1	l.6 1.5 1	1.5
С С	OTFG7/CASTEP	2.5 2.5	2.6 2	2.6 2.5	2.6 5.8	3.1	2.9 3.0	3.8	3.8 2.5	5 2.8	5.6	2.5	2.7 3.	0 2.6	3.1	2.2 3	3.5 2.	.5 2.6	2.6	2.6 2	6	2.2 2	2.4 4.8	5.7	14.5	2.7 2.9	9 3.4	2.4 2	2.6 2.6 2	2.6
US	OTFG9/CASTEP	0.4 0.5	0.7 0	0.7 0.5	0.7 4.1	1.1	1.0 1.0	0 1.8	2.0 0.5	5 1.0	3.9	1.4	1.5 1.4	4 0.7	1.6	0.9 2	2.1 0.	.8 0.5	1.0	0.9 1	0 2.2	(0.6 6.3	6.2	13.6	2.2 1.3	L 2.1	0.8 1	L.5 1.4 1	1.5
	SSSP/QE	0.4 0.3	0.6 0).6 0.3	0.5 3.9	1.0	0.9 0.8	3 1.6	1.7 0.3	8 0.7	3.6	1.3	1.4 1.	1 0.6	1.5	0.7 1	L.9 0.	.6 0.4	0.8	0.9 0	8 2.4	0.6	6.4	6.2	13.6	2.1 1.0	2.0	0.7 1	1.4 1.2 1	1.3
	Vdb/CASTEP	6.4 6.4	6.4 6	6.5 6.4	6.5 7.9	6.6	6.4 6.	7 7.1	6.9 6.4	6.4	7.4	6.5	6.5 6.	5 6.3	6.1	6.1 6	6.5 6.	.5 6.6	6.3	6.2 6	3 4.8	6.3 6	5.4	9.6	16.3	6.6 6.3	L 6.6	6.4 5	5.7 5.8 5	5.7
	Vdb2/DACAPO	6.3 6.3	6.3 6	6.3 6.3	6.3 7.2	6.4	6.4 6.	5 7.0	6.9 6.2	2 6.3	7.6	6.1	6.1 6.	5 6.2	5.8	5.9 6	6.1 6.	.3 6.2	6.4	6.3 6	3 5.7	6.2 6	5.2 9.6		17.9	6.2 5.9	9 6.4	6.1 6	6.5 6.5 6	6.5
	FHI98pp/ABINIT	13.5 13.4	13.6 13	3.6 13.4	13.2 13.0) 13.7	13.0 13.	2 13.0	12.3 13.	4 15.1	12.3	13.6 1	.3.6 13	0 13.4	4 12.8	13.5 12	2.4 13	8.4 13.7	15.3	15.0 15	.2 14.5	13.6 1	3.6 16.3	8 17.9	1	.4.3 8.5	5 13.0	13.3 13	3.3 13.6 1	.3.4
-		2.2 2.2																											2.0 2.0 2	
РР	_	1.1 1.1																											l.5 1.4 1	
Ŭ	_	2.1 2.1																											2.2 2.2 2	
Ž		0.7 0.7																											L.3 1.4 1	
	ONCVPSP(SG15)1/CASTEP	1.5 1.4																											0.3 (
	ONCVPSP(SG15)1/QE																													0.3
	ONCVPSP(SG15)2/CASTEP	1.4 1.4	1.5 1	1.5 1.4	1.3 4.1	1.6	1.6 1.	5 2.1	1.9 1.4	1.8	3.7	1.7 :	1.8 1.4	4 1.4	2.1	1.6 2	2.5 1.	6 1.5	1.6	1.5 1	5 2.6	1.5 1	l.3 <u>5</u> .7	6.5	13.4	2.0 1.4	1 2.2	1.3 0	.1 0.3	

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DFT codes using PAW

- VASP license
- <u>Abinit free</u>
- <u>Quantum Espresso</u> free
- <u>GPAW</u> free
- + more



Importance of good potential database

Refs.

- Good presentations by <u>Marsman</u> and <u>Blöchl</u>
- Blöchl PRB 50, 17953 (1994)
- Blöchl et al. <u>https://arxiv.org/abs/cond-mat/0201015v2</u>
- Kresse & Joubert PRB 59, 1758 (1999)
- Holzwarth et al. PRB 55, 2005 (1997)
- Martin, *Electronic Structure*, Chapter 11.1, 13.2

