VASP - Best Practices Workshop

Weine Olovsson

National Supercomputer Centre (NSC), Linköping University

SNIC-PRACE training, online @NSC 19-20th Oct 2020

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VASP - Best Practices Workshop

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

https://www.snic.se/

https://training.prace-ri.eu/

National Supercomputer Centre (NSC)

NSC is part of:

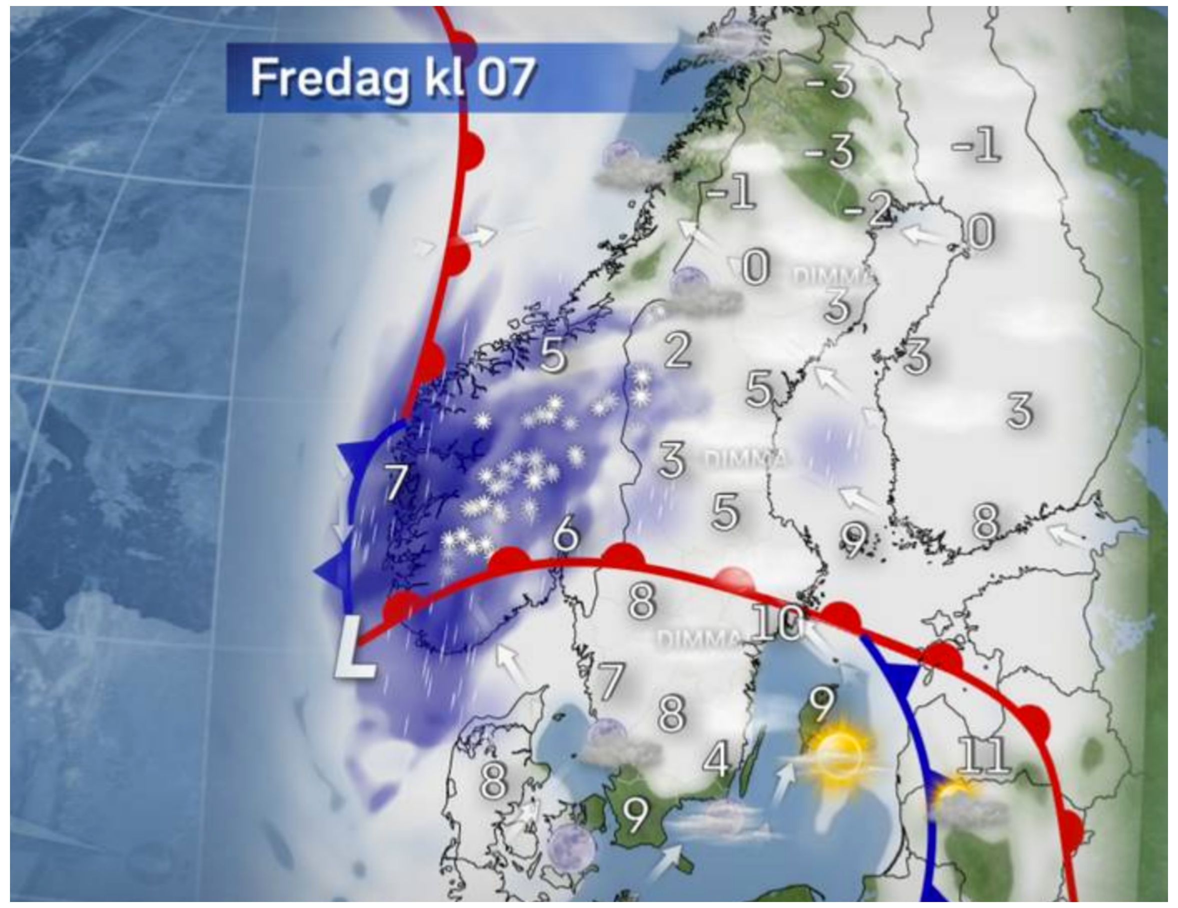
- SNIC Swedish National Infrastructure for Computing (10 Univ.)
- LiU LINKÖPING UNIVERSITY liu.se

NSC partners: SAAB, SMHI, MET Norway

SMHI

Meteorologisk institutt

SAAB



NSC academic clusters

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

SNIC

Top500 no. 95 (74)

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

LINKÖPING UNIVERSITY

BerzeLiUs (2021 -) Nvidia DGX SuperPOD, 60 x 8 A100 GPUs

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Knut and Alice Wallenberg Foundation

About myself

- 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, GPAW, WIEN2k, …

Information / Schedule

https://www.nsc.liu.se/support/Events/VASP_workshop_2020/

Monday 19th Oct

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

Tuesday 20th Oct

10:00 -11:00 Running & Performance
11:00 -12:00 Cont., Utilities & Summary
12:00 -13:00 Lunch
13:00 -15:00 Hands-on session (guided)
15:00 -17:00 Hands-on session

10-15 min breaks every hour

Workshop organization

- Weine Olovsson - presentation
- Diana Iusan (UPPMAX) - helper seminar & hands-on
- Peter Kjellström - helper hands-on
- Hamish Struthers - helper hands-on
- support@nsc.liu.se - help with accounts

VASP - Best Practices Workshop

- Basic theory (PAW)
- General considerations

...at specific supercomputer centres

- Focus on practical aspects of running VASP
- Influential parameters, NPAR/NCORE, ALGO, NSIM, KPAR, …
- Benchmarks, examples
- Common problems

… clickable links are underlined

Resources

- Wiki / Manual

  Check in detail!

- Wiki

  examples, presentations

- Forum

Find the links:

http://vasp.at/

- Peter Larsson's (old) blog at NSC:

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

info & discussion

Questions/trouble? support@nsc.liu.se, …

1. Introduction & Basic Theory

Weine Olovsson

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VASP - Best Practices Workshop

NSC SNIC PRACE

https://www.nsc.liu.se/ https://www.snic.se/ https://training.prace-ri.eu/

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 underlined

http://vasp.at/

Schrödinger Equation

Time-independent SE

$$H\Psi = E\Psi,$$

Born-Oppenheimer approx.
= 0

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

solid ~10^{23} particles…

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(**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(**r**)

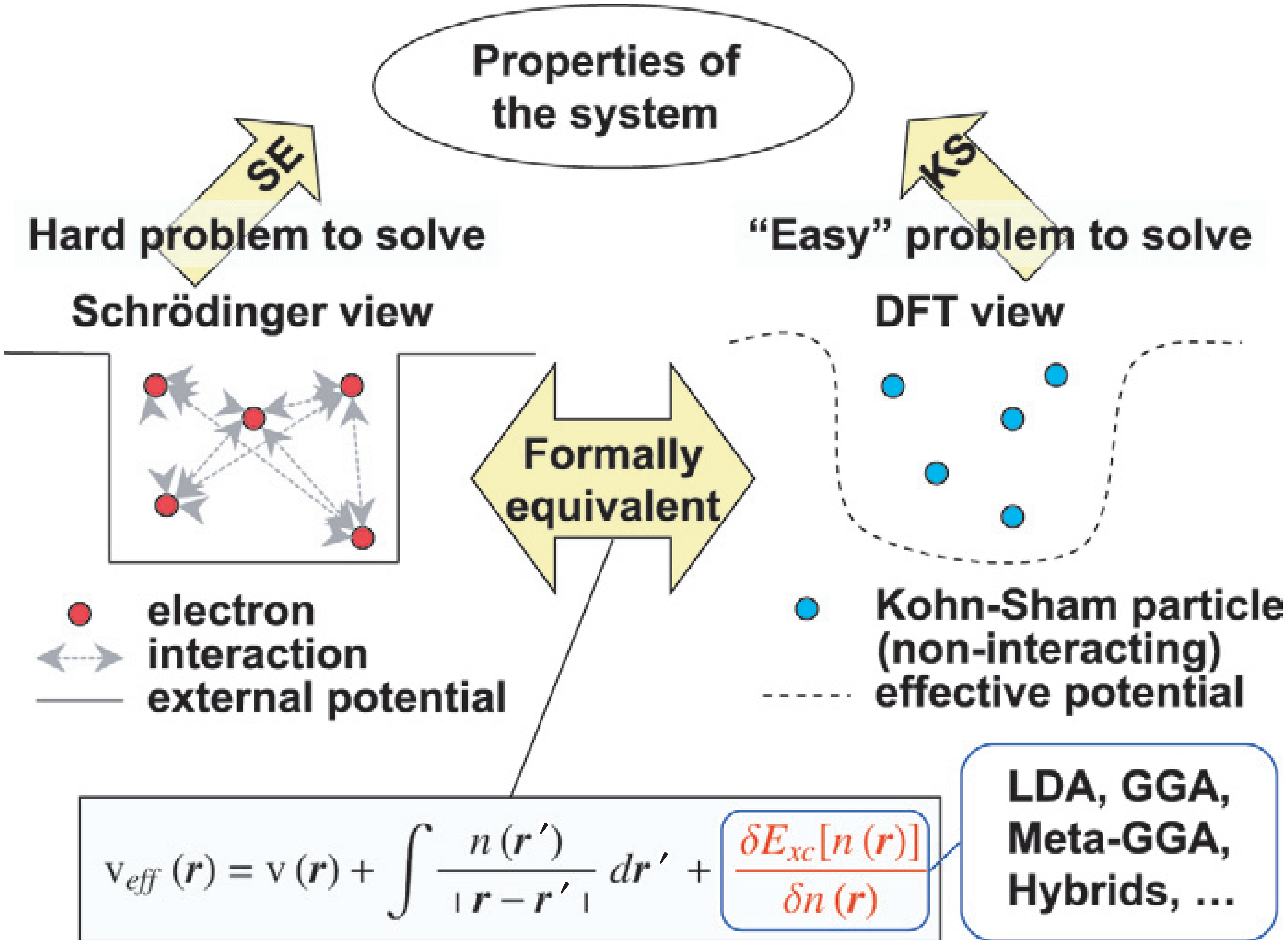
(2) The total energy functional E[n], for a given V_{ext}, assumes its minimal value for the correct electron density n(**r**) of the ground state

Ansatz:

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

for *independent* electrons (mean field theory)

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



$$v_{eff}(\mathbf{r}) = v(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}' + \frac{\delta E_{xc}[n(\mathbf{r})]}{\delta n(\mathbf{r})}$$

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…

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

Local Density Approximation (LDA)

homogeneous electron gas

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

Generalized Gradient Approximation (GGA)

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

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

Using periodicity

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

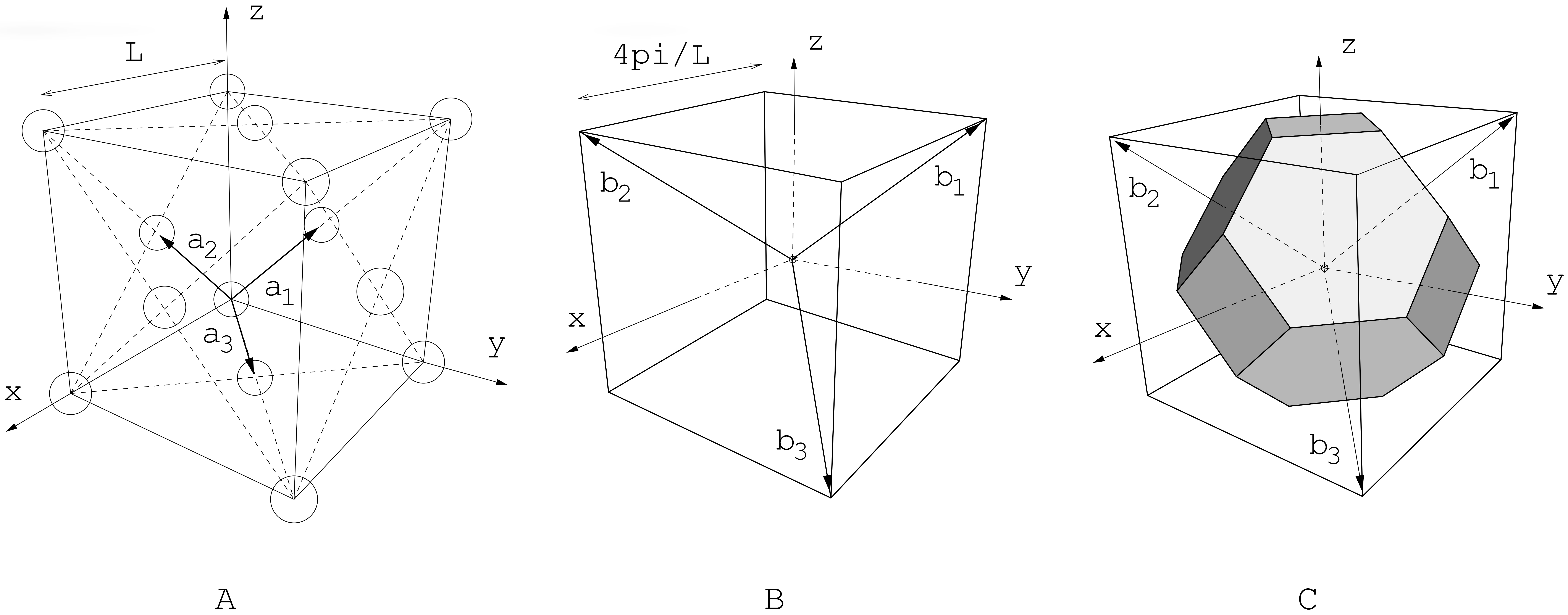
  $$\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = \psi_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{kR}}$$

  where $\mathbf{R}$ is any translational vector leaving the Hamiltonian invariant.
- $\mathbf{k}$ 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: https://www.vasp.at/mmars/day1.pdf

Using periodicity

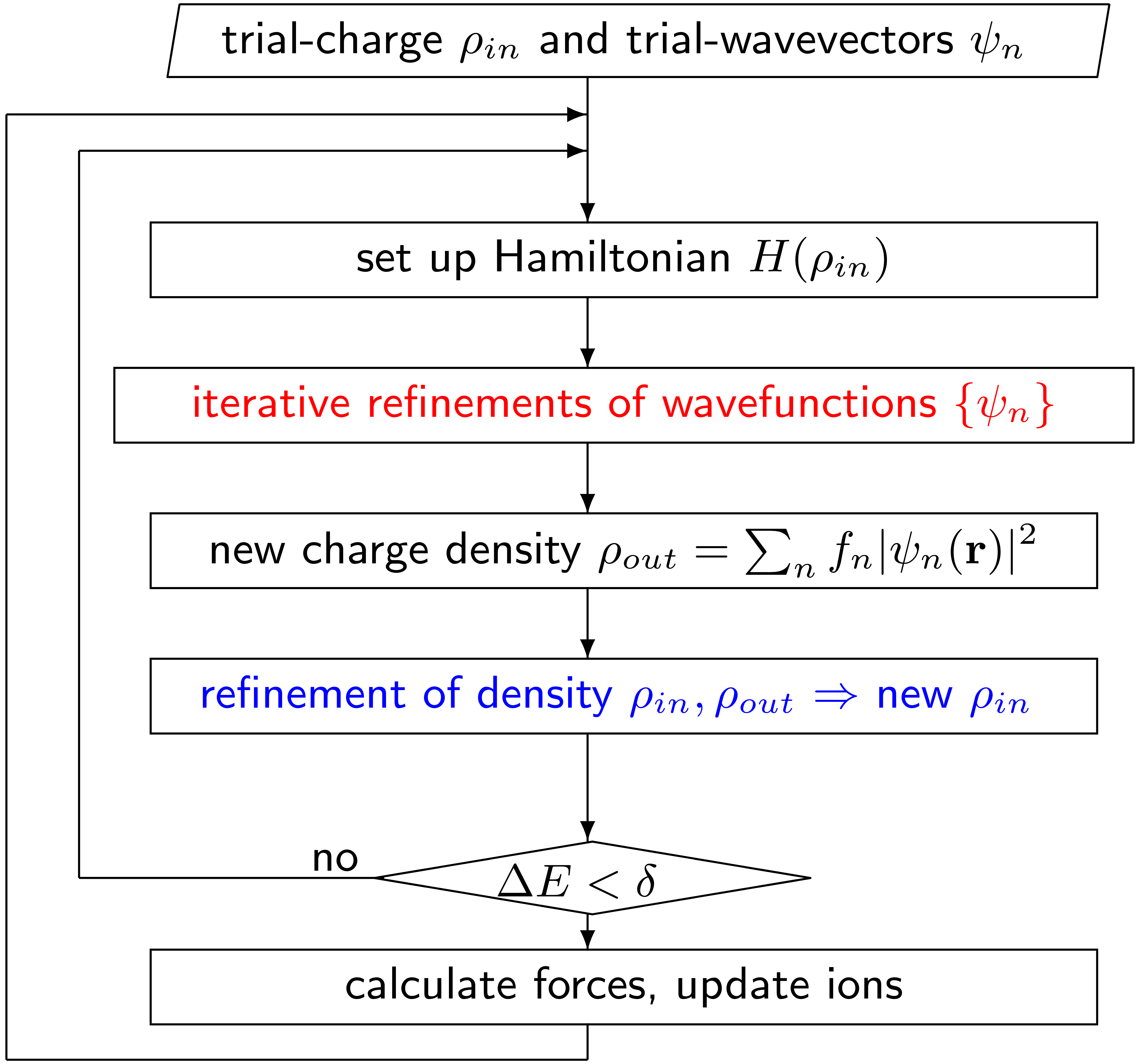


$$\mathbf{b}_1 = \frac{2\pi}{\Omega}\mathbf{a}_2 \times \mathbf{a}_3 \quad \mathbf{b}_2 = \frac{2\pi}{\Omega}\mathbf{a}_3 \times \mathbf{a}_1 \quad \mathbf{b}_3 = \frac{2\pi}{\Omega}\mathbf{a}_1 \times \mathbf{a}_2$$

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

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

Self-consistent iterations



- 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

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

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

therefore ->

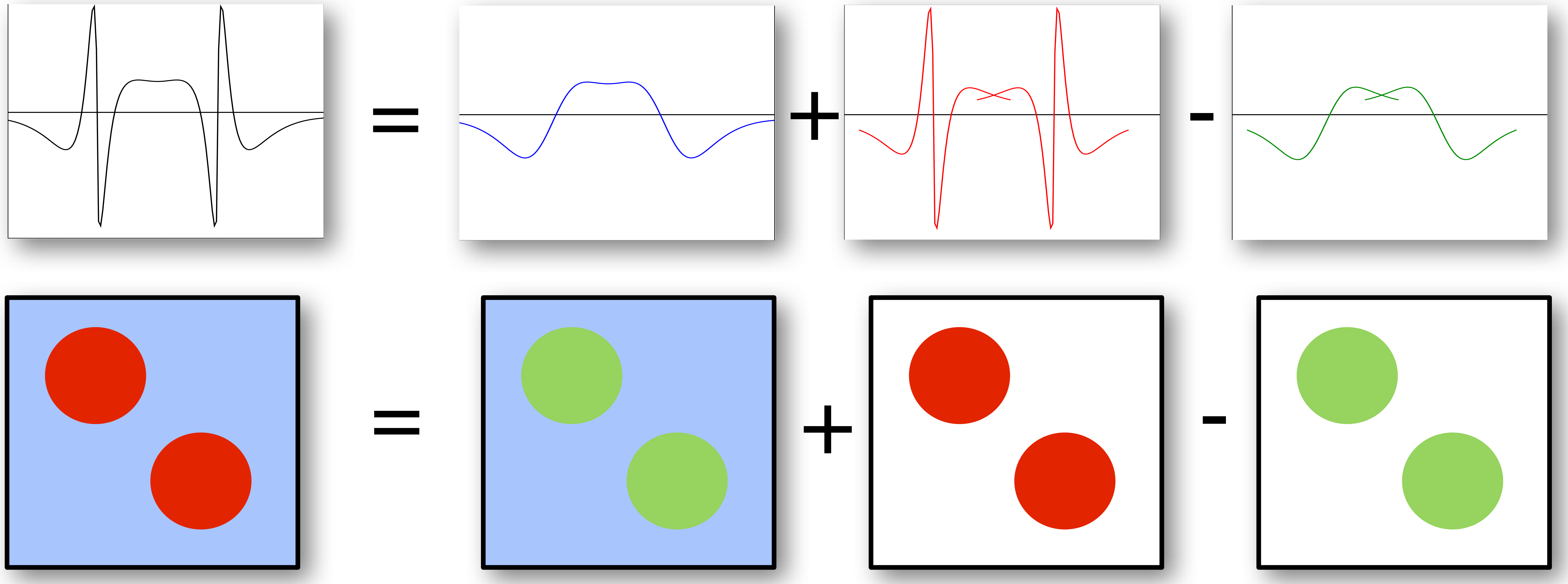
- Split into *interstitial* and *augmentation* (sphere) regions

smooth pw

- No overlap between spheres (one-centre expansion)
- PAW: Energy and potential *independent* wave functions

PAW Augmentation

$$\underbrace{|\psi\rangle}_{\text{all-electron}} = \overbrace{|\tilde{\psi}\rangle}^{\text{pseudo}} + \overbrace{\underbrace{|\psi^1\rangle}_{\text{1-center, all-el.}}}^{\sum_\alpha |\phi_\alpha\rangle\langle\tilde{p}_\alpha|\tilde{\psi}\rangle} - \overbrace{\underbrace{|\tilde{\psi}^1\rangle}_{\sum_\alpha |\tilde{\phi}_\alpha\rangle\langle\tilde{p}_\alpha|\tilde{\psi}\rangle}}^{\text{1-center, pseudo}}$$



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

Transformation theory

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

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

Kohn-Sham equation:

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

Can write Schrödinger-like equation:

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

$$\langle A\rangle \quad = \quad \sum_n f_n\langle\Psi_n|A|\Psi_n\rangle = \sum_n f_n\langle\tilde{\Psi}_n|\mathcal{T}^\dagger A\mathcal{T}|\tilde{\Psi}_n\rangle$$

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

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

Transformation operator

$$\mathcal{T} = 1 + \sum_R \mathcal{S}_R$$

TO unity in *interstitial*, outside *augmentation sphere* R

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

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

$$\begin{aligned} |\phi_i\rangle &= (1 + S_R)|\tilde{\phi}_i\rangle \quad \text{for} \quad i \in R \\ S_R|\tilde{\phi}_i\rangle &= |\phi_i\rangle - |\tilde{\phi}_i\rangle \end{aligned}$$

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

$$\tilde{\Psi}(\mathbf{r}) = \sum_{i\in R} \tilde{\phi}_i(\mathbf{r}) \langle \tilde{p}_i | \tilde{\Psi} \rangle \quad \text{for} \quad |\mathbf{r} - \mathbf{R}_R| < r_{c,R}$$

Expand PS wf in PS partial waves

projector function

$$\langle \tilde{p}_i | \tilde{\phi}_j \rangle = \delta_{i,j} \quad \text{for} \quad i, j \in R$$

requirement for above to hold

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

Transformation operator

$$S_R|\tilde{\Psi}\rangle = \sum_{i\in R} S_R|\tilde{\phi}_i\rangle\langle\tilde{p}_i|\tilde{\Psi}\rangle = \sum_{i\in R}\Big(|\phi_i\rangle - |\tilde{\phi}_i\rangle\Big)\langle\tilde{p}_i|\tilde{\Psi}\rangle$$

From using the previous relations

$$\mathcal{T} = 1 + \sum_i \Big(|\phi_i\rangle - |\tilde{\phi}_i\rangle\Big)\langle\tilde{p}_i|$$

Final expression for the transformation operator

$$\boxed{|\Psi\rangle = |\tilde{\Psi}\rangle + \sum_i \Big(|\phi_i\rangle - |\tilde{\phi}_i\rangle\Big)\langle\tilde{p}_i|\tilde{\Psi}\rangle = |\tilde{\Psi}_n\rangle + \sum_R \Big(|\Psi_R^1\rangle - |\tilde{\Psi}_R^1\rangle\Big)}$$

$$|\Psi_R^1\rangle = \sum_{i\in R} |\phi_i\rangle\langle\tilde{p}_i|\tilde{\Psi}\rangle$$

$$|\tilde{\Psi}_R^1\rangle = \sum_{i\in R} |\tilde{\phi}_i\rangle\langle\tilde{p}_i|\tilde{\Psi}\rangle$$

Final expression for the *true* AE wf:

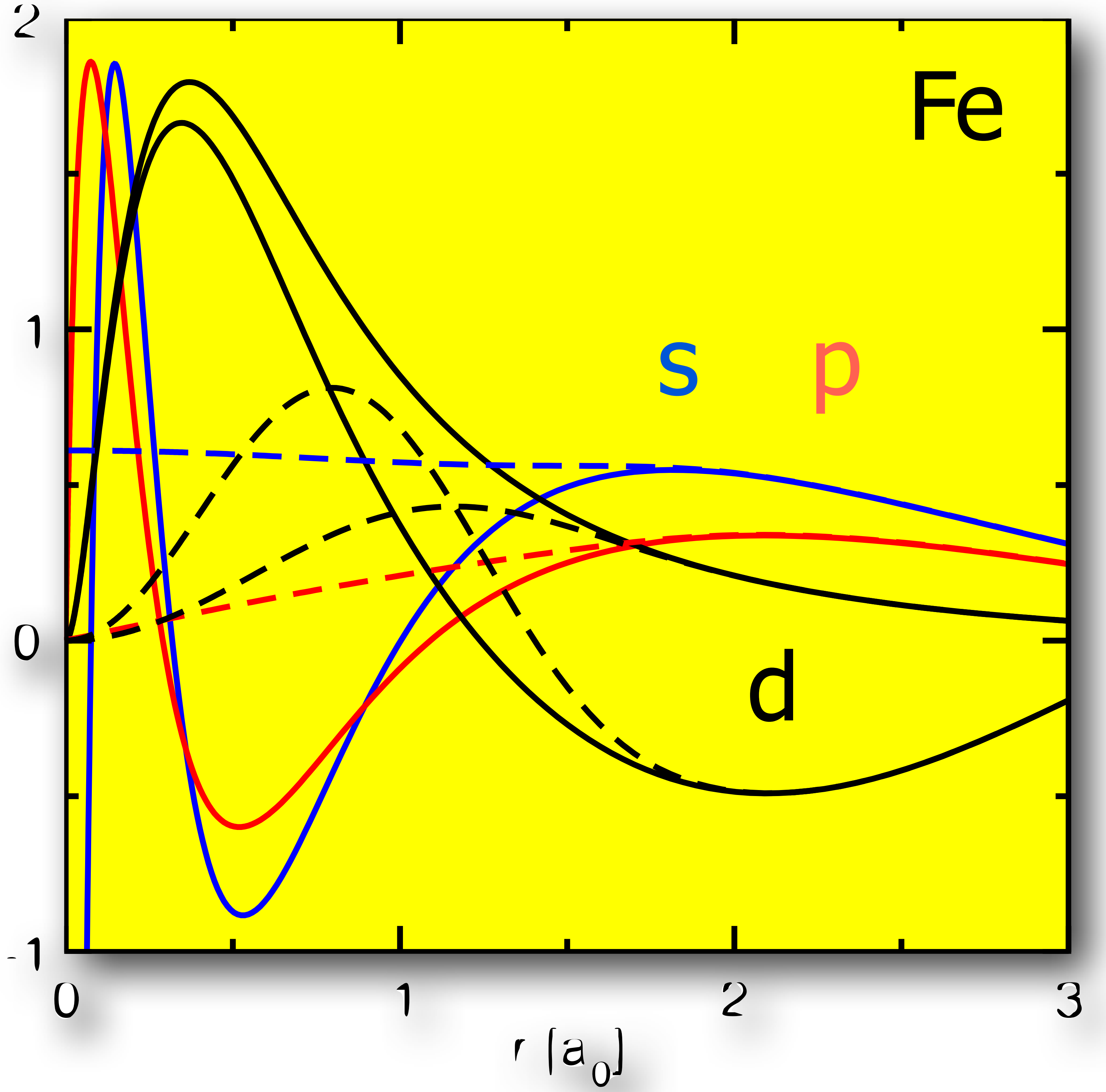
- one PS wf expanded in plane waves

- two atom centred localised functions

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

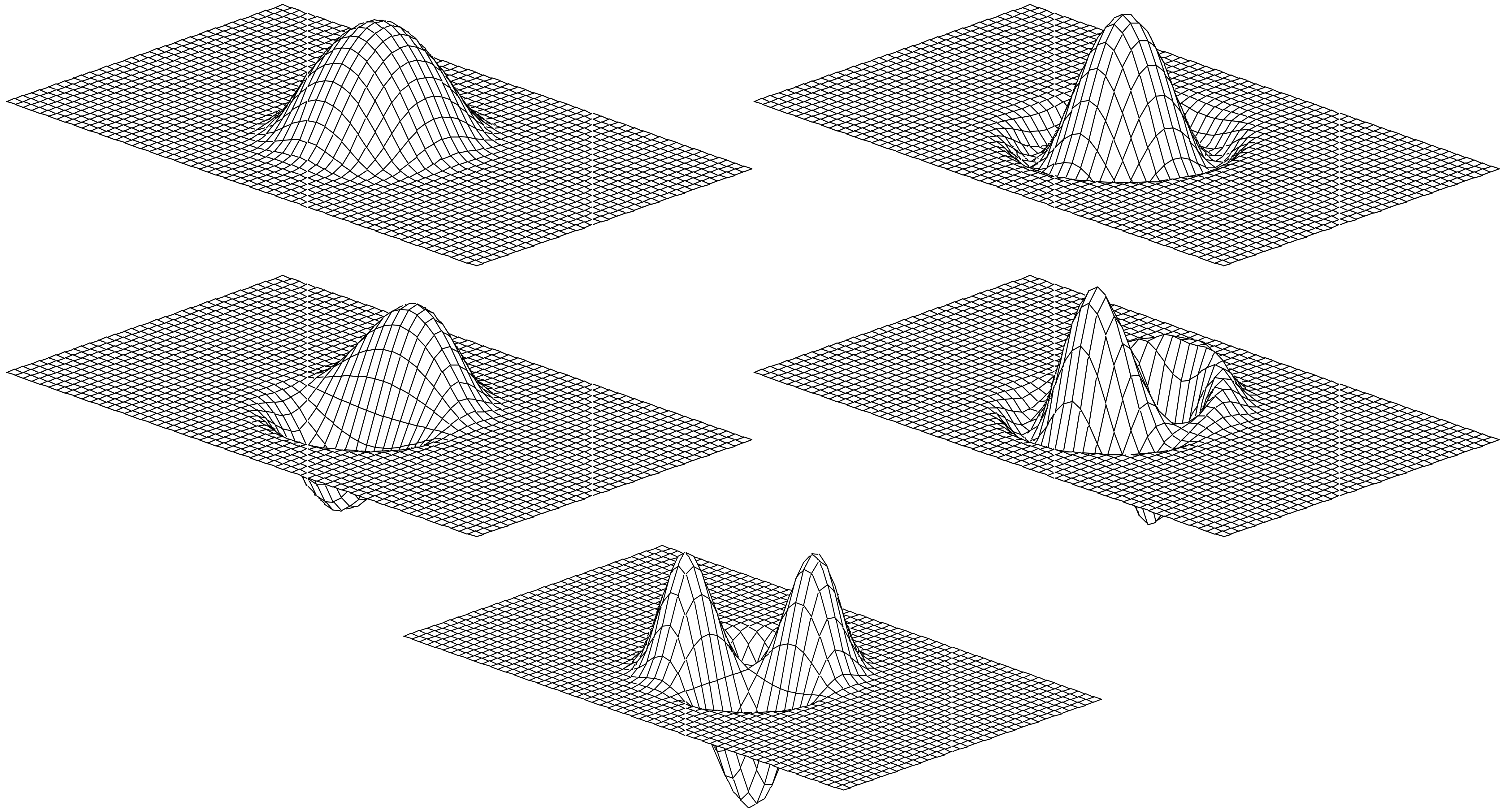
Partial waves

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



- Localised
- Angular momentum of partial waves

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

Wave functions

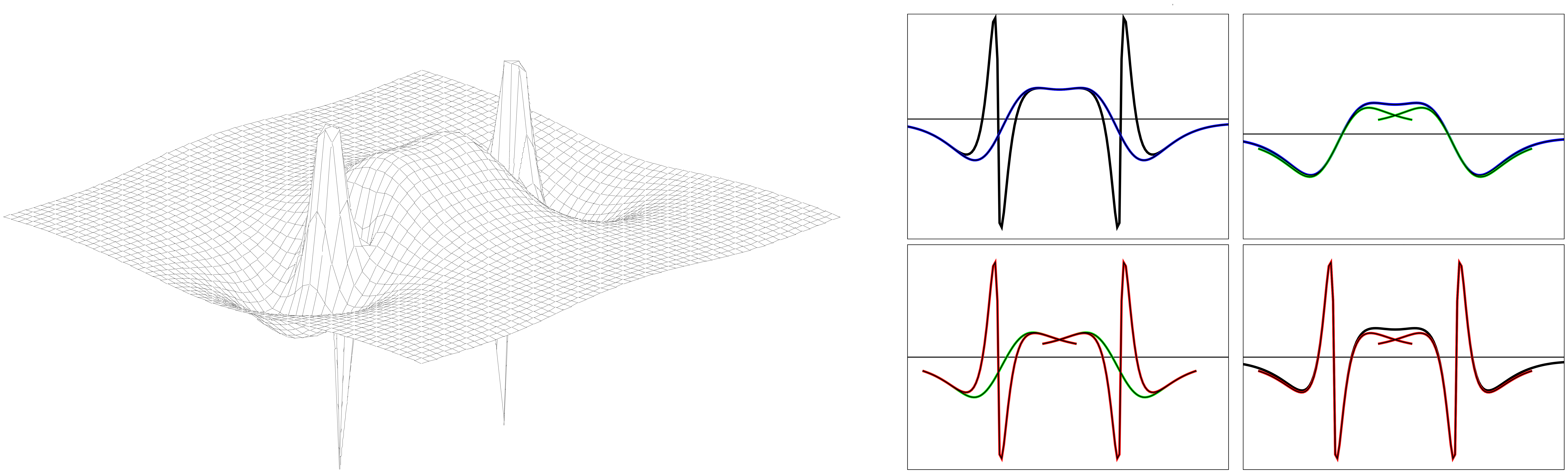


Figure 2: Bonding p-σ orbital of the Cl_2 molecule and its decomposition of the wave function into auxiliary wave function and the two one-center expansions. Top-left: True and auxiliary wave function; top-right: auxiliary wave function and its partial wave expansion; bottom-left: the two partial wave expansions; bottom-right: true wave function and its partial wave expansion.

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

More examples

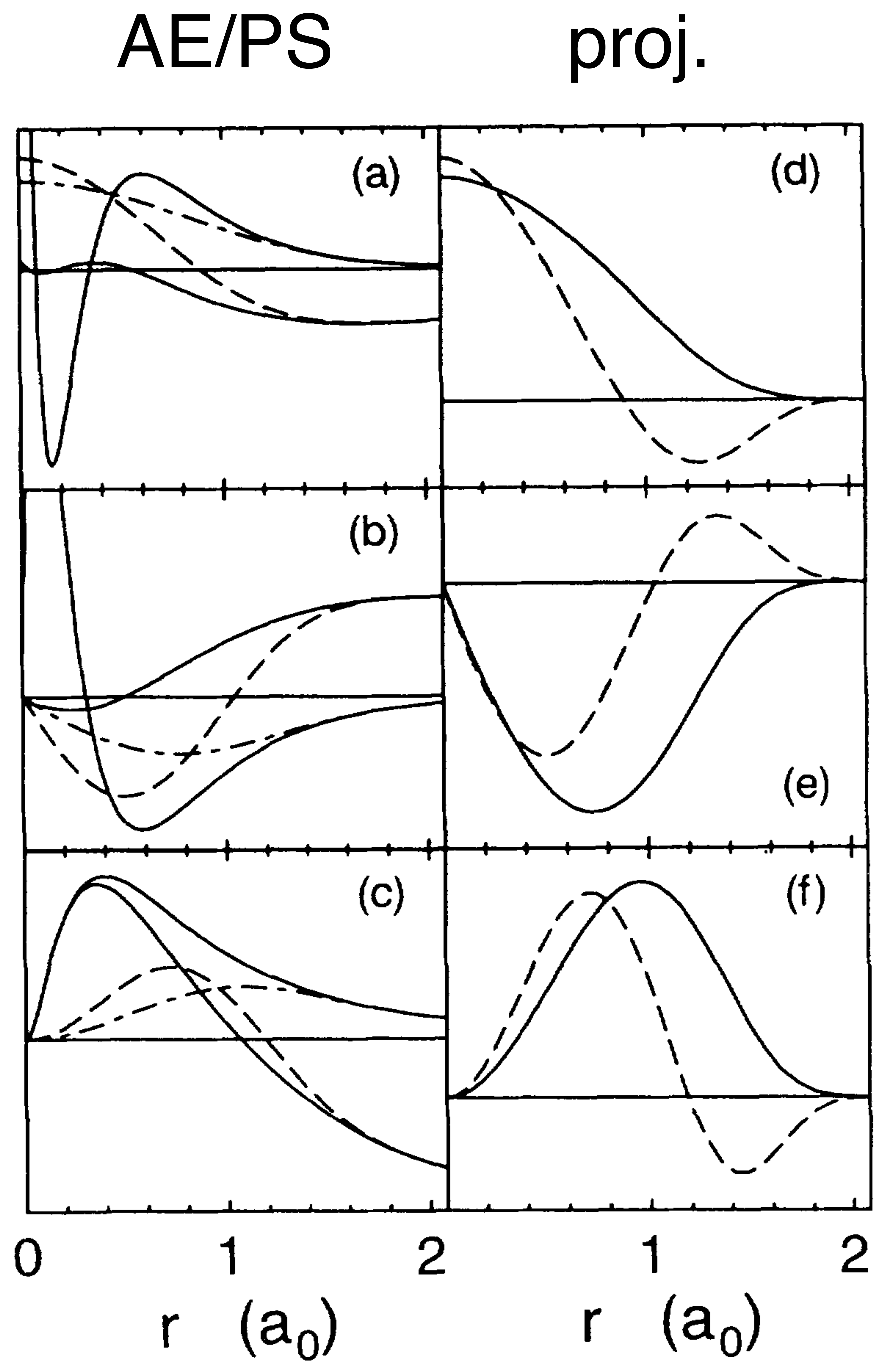
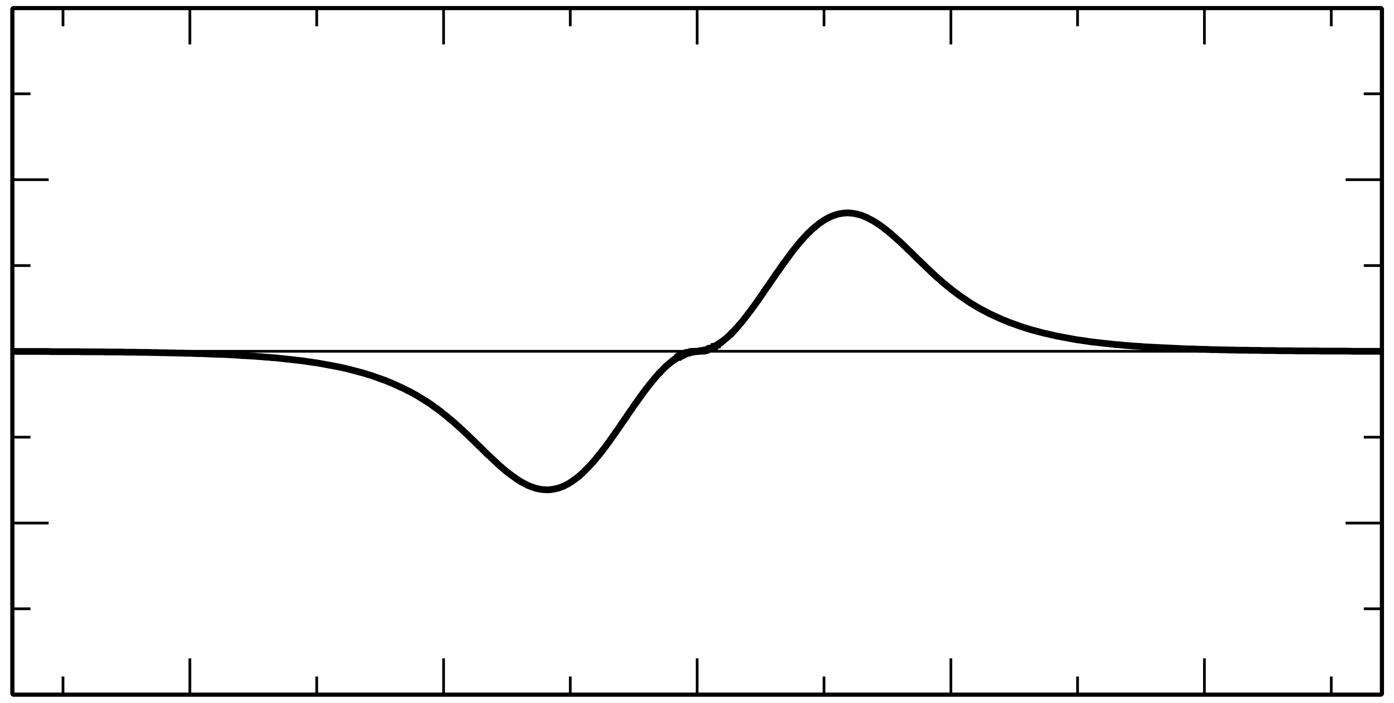


FIG. 1. Partial waves and projectors for Mn. Left panel: AE partial waves (solid lines) and PS partial waves (dashed and dash-dotted lines). The "first" PS partial wave is a dash-dotted line. Right panel: first (solid line) and second (dashed line) projector functions. (a) and (d) show the results for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

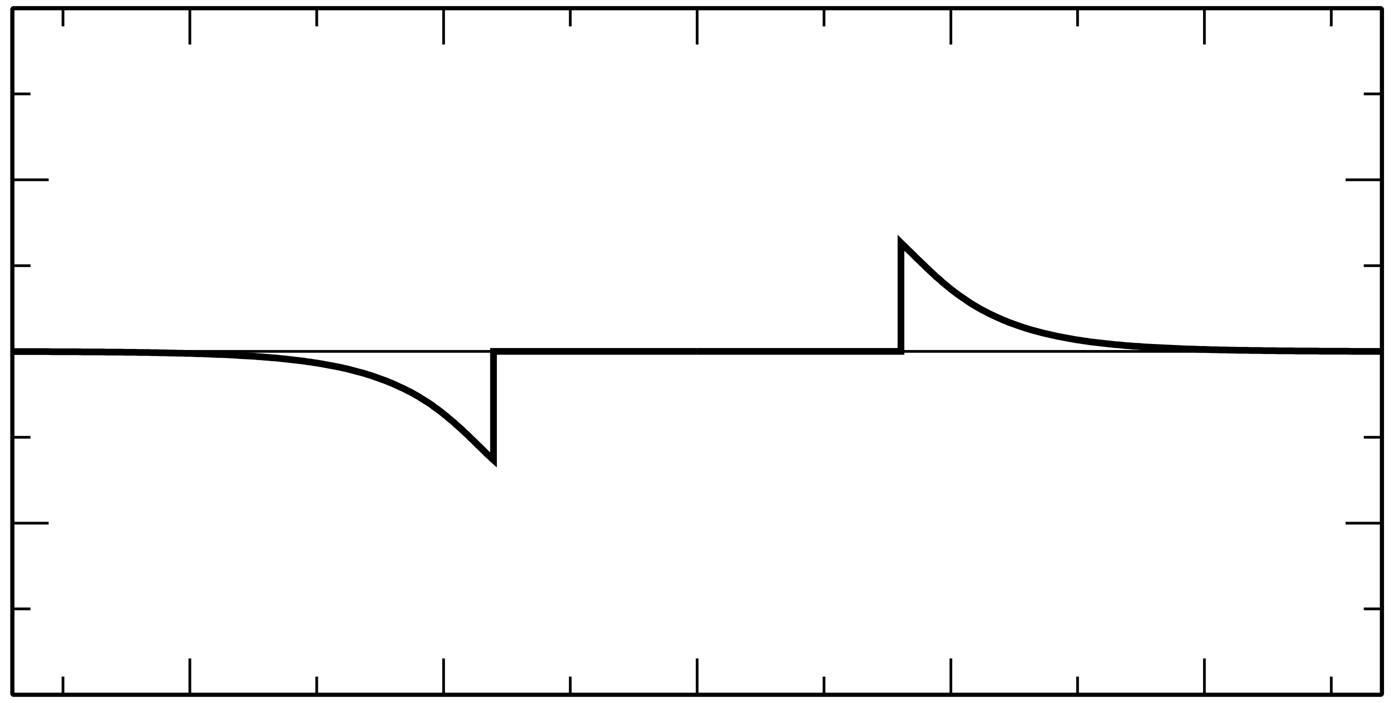
Blöchl PRB 50, 17953 (1994)

PAW Augmentation

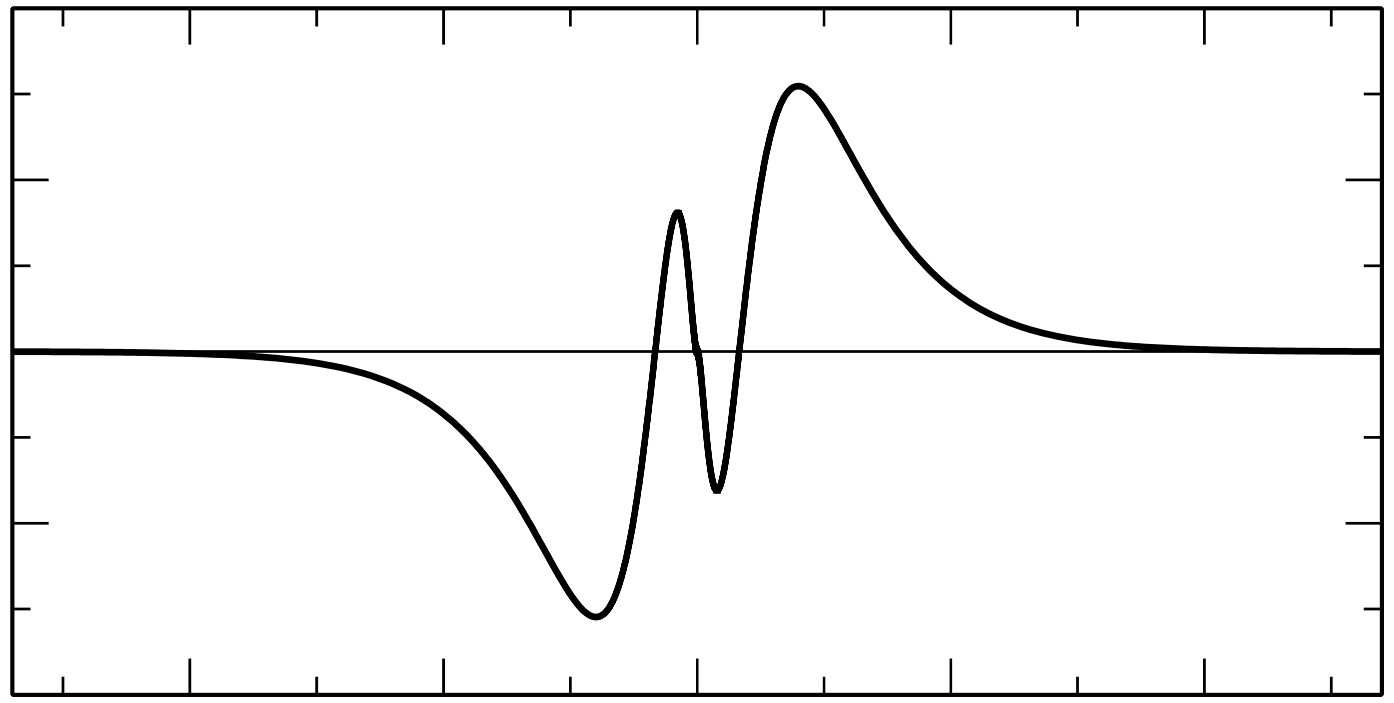
$$|\widetilde{\psi}_n\rangle$$



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



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

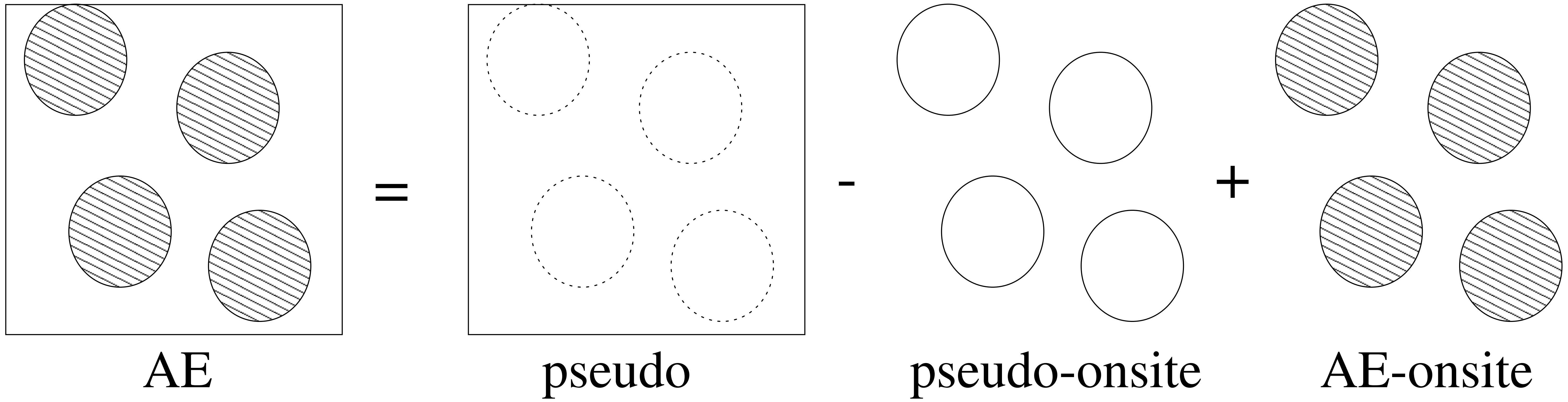


from Marsman: https://www.vasp.at/mmars/day1.pdf

PAW Augmentation

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

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



- Same trick works for
  - Wavefunctions
  - Charge density
  - Kinetic energy
  - Exchange correlation energy
  - Hartree energy

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

Total Energy

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

three terms

$$\tilde{E} = \sum_n f_n \langle\tilde{\psi}_n| -\frac{1}{2}\Delta|\tilde{\psi}_n\rangle + E_{xc}[\tilde{\rho}+\hat{\rho}+\tilde{\rho}_c] + E_H[\tilde{\rho}+\hat{\rho}] + \int v_H[\tilde{\rho}_{Zc}]\,(\tilde{\rho}(\mathbf{r})+\hat{\rho}(\mathbf{r}))\;d^3\mathbf{r} + \;U(\mathbf{R},Z_{\text{ion}})$$

PW grid

$$\tilde{E}^1 = \sum_{\text{sites}}\left\{\sum_{(i,j)}\rho_{ij}\langle\tilde{\phi}_i| -\frac{1}{2}\Delta|\tilde{\phi}_j\rangle + \overline{E_{xc}[\tilde{\rho}^1+\hat{\rho}+\tilde{\rho}_c]} + \overline{E_H[\tilde{\rho}^1+\hat{\rho}]} + \int_{\Omega_r} v_H[\tilde{\rho}_{Zc}]\,\left(\tilde{\rho}^1(\mathbf{r})+\hat{\rho}(\mathbf{r})\right)\;d^3\mathbf{r}\right\}$$

local
radial grid

$$E^1 = \sum_{\text{sites}}\left\{\sum_{(i,j)}\rho_{ij}\langle\phi_i| -\frac{1}{2}\Delta|\phi_j\rangle + \overline{E_{xc}[\rho^1+\rho_c]} + \overline{E_H[\rho^1]} + \int_{\Omega_r} v_H[\rho_{Zc}]\rho^1(\mathbf{r})\,d^3\mathbf{r}\right\}$$

local
radial grid

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

What are the approximations?

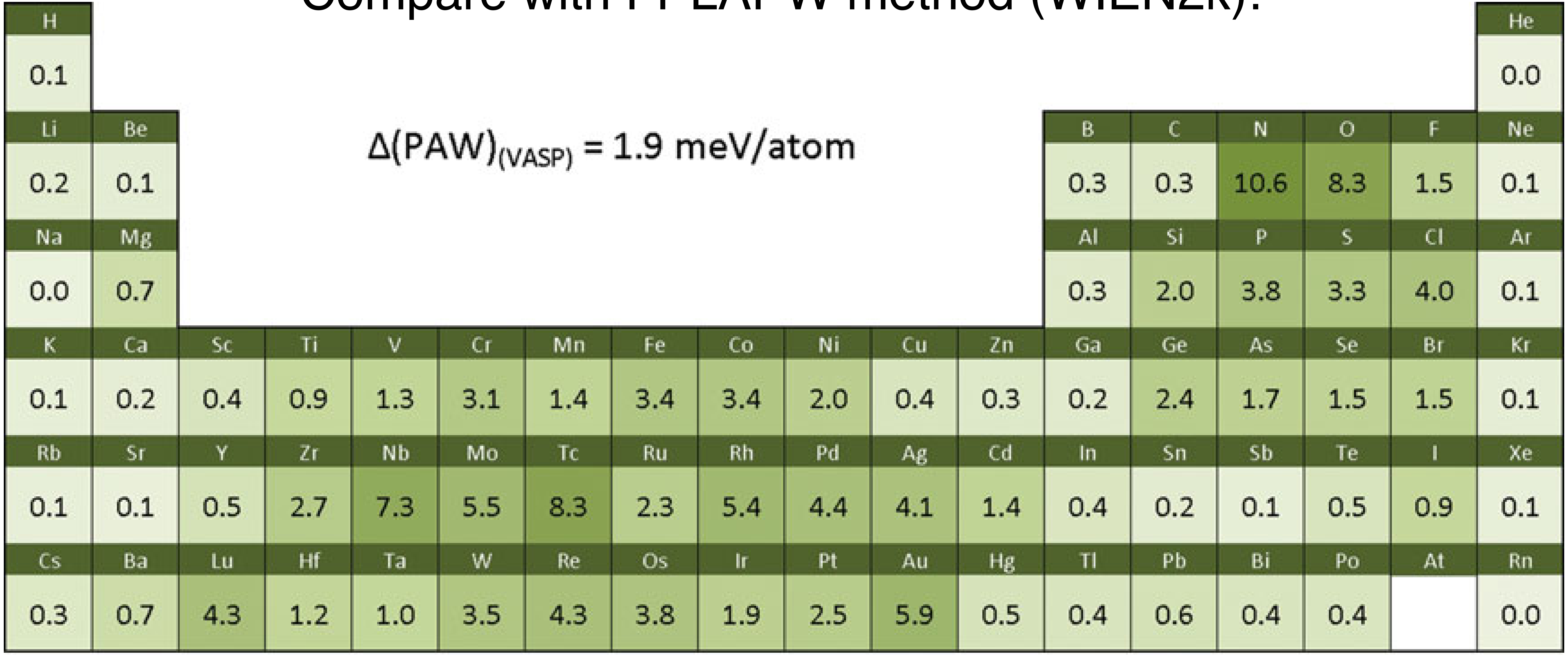
- Frozen core can be relaxed: Marsman & Kresse, JCP 125, 104101 (2006)
- Plane wave expansion, energy cut-off $\frac{1}{2}|\mathbf{G}+\mathbf{k}|^2 < E_{\text{cutoff}}$
- Partial wave expansion (1-2 per angular momentum)

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):

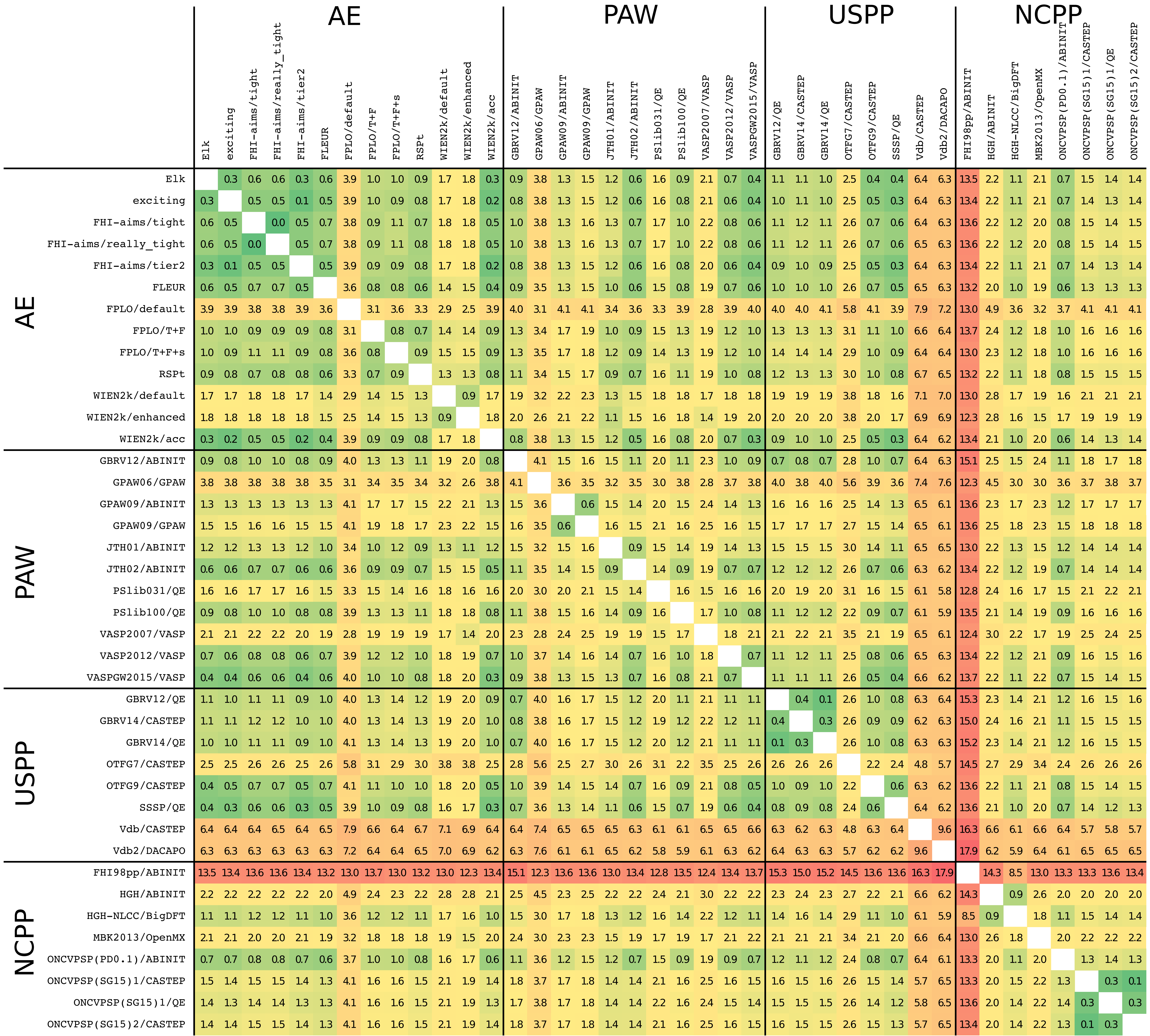


$\Delta(\mathrm{PAW})_{(\mathrm{VASP})} = 1.9$ meV/atom

H																	He
0.1																	0.0
Li	Be											B	C	N	O	F	Ne
0.2	0.1											0.3	0.3	10.6	8.3	1.5	0.1
Na	Mg											Al	Si	P	S	Cl	Ar
0.0	0.7											0.3	2.0	3.8	3.3	4.0	0.1
K	Ca	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	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.1	0.1	0.5	2.7	7.3	5.5	8.3	2.3	5.4	4.4	4.1	1.4	0.4	0.2	0.1	0.5	0.9	0.1
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	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)

Lejaeghere et al. Science 351, 1415 (2016)



		AE													PAW											USPP								NCPP							
		Elk	exciting	FHI-aims/tight	FHI-aims/really_tight	FHI-aims/tier2	FLEUR	FPLO/default	FPLO/T+F	FPLO/T+F+s	RSPt	WIEN2k/default	WIEN2k/enhanced	WIEN2k/acc	GBRV12/ABINIT	GPAW06/GPAW	GPAW09/ABINIT	GPAW09/GPAW	JTH01/ABINIT	JTH02/ABINIT	PSlib031/QE	PSlib100/QE	VASP2007/VASP	VASP2012/VASP	VASPGW2015/VASP	GBRV12/QE	GBRV14/CASTEP	GBRV14/QE	OTFG7/CASTEP	OTFG9/CASTEP	SSSP/QE	Vdb/CASTEP	Vdb2/DACAPO	FHI98pp/ABINIT	HGH/ABINIT	HGH-NLCC/BigDFT	MBK2013/OpenMX	ONCVPSP(PD0.1)/ABINIT	ONCVPSP(SG15)1/CASTEP	ONCVPSP(SG15)1/QE	ONCVPSP(SG15)2/CASTEP
AE	Elk		0.3	0.6	0.6	0.3	0.6	3.9	1.0	1.0	0.9	1.7	1.8	0.3	0.9	3.8	1.3	1.5	1.2	0.6	1.6	0.9	2.1	0.7	0.4	1.1	1.1	1.0	2.5	0.4	0.4	6.4	6.3	13.5	2.2	1.1	2.1	0.7	1.5	1.4	1.4
	exciting	0.3		0.5	0.5	0.1	0.5	3.9	1.0	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	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	1.1	2.1	0.7	1.4	1.3	1.4
	FHI-aims/tight	0.6	0.5		0.0	0.5	0.7	3.8	0.9	1.1	0.7	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.4	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
	FHI-aims/really_tight	0.6	0.5	0.0		0.5	0.7	3.8	0.9	1.1	0.8	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.5	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
	FHI-aims/tier2	0.3	0.1	0.5	0.5		0.5	3.9	0.9	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.0	0.6	0.4	0.9	1.0	0.9	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
	FLEUR	0.6	0.5	0.7	0.7	0.5		3.6	0.8	0.8	0.6	1.4	1.5	0.4	0.9	3.5	1.3	1.5	1.0	0.6	1.5	0.8	1.9	0.7	0.6	1.0	1.0	1.0	2.6	0.7	0.5	6.5	6.3	13.2	2.0	1.0	1.9	0.6	1.3	1.3	1.3
	FPLO/default	3.9	3.9	3.8	3.8	3.9	3.6		3.1	3.6	3.3	2.9	2.5	3.9	4.0	3.1	4.1	4.1	3.4	3.6	3.3	3.9	2.8	3.9	4.0	4.0	4.0	4.1	5.8	4.1	3.9	7.9	7.2	13.0	4.9	3.6	3.2	3.7	4.1	4.1	4.1
	FPLO/T+F	1.0	1.0	0.9	0.9	0.9	0.8	3.1		0.8	0.7	1.4	1.4	0.9	1.3	3.4	1.7	1.9	1.0	0.9	1.5	1.3	1.9	1.2	1.0	1.3	1.3	1.3	3.1	1.1	1.0	6.6	6.4	13.7	2.4	1.2	1.8	1.0	1.6	1.6	1.6
	FPLO/T+F+s	1.0	0.9	1.1	1.1	0.9	0.8	3.6	0.8		0.9	1.5	1.5	0.9	1.3	3.5	1.7	1.8	1.2	0.9	1.4	1.3	1.9	1.2	1.0	1.4	1.4	1.4	2.9	1.0	0.9	6.4	6.4	13.0	2.3	1.2	1.8	1.0	1.6	1.6	1.6
	RSPt	0.9	0.8	0.7	0.8	0.8	0.6	3.3	0.7	0.9		1.3	1.3	0.8	1.1	3.4	1.5	1.7	0.9	0.7	1.6	1.1	1.9	1.0	0.8	1.2	1.3	1.3	3.0	1.0	0.8	6.7	6.5	13.2	2.2	1.1	1.8	0.8	1.5	1.5	1.5
	WIEN2k/default	1.7	1.7	1.8	1.8	1.7	1.4	2.9	1.4	1.5	1.3		0.9	1.7	1.9	3.2	2.2	2.3	1.3	1.5	1.8	1.8	1.7	1.8	1.8	1.9	1.9	1.9	3.8	1.8	1.6	7.1	7.0	13.0	2.8	1.7	1.9	1.6	2.1	2.1	2.1
	WIEN2k/enhanced	1.8	1.8	1.8	1.8	1.8	1.5	2.5	1.4	1.5	1.3	0.9		1.8	2.0	2.6	2.1	2.2	1.1	1.5	1.6	1.8	1.4	1.9	2.0	2.0	2.0	2.0	3.8	2.0	1.7	6.9	6.9	12.3	2.8	1.6	1.5	1.7	1.9	1.9	1.9
	WIEN2k/acc	0.3	0.2	0.5	0.5	0.2	0.4	3.9	0.9	0.9	0.8	1.7	1.8		0.8	3.8	1.3	1.5	1.2	0.5	1.6	0.8	2.0	0.7	0.3	0.9	1.0	1.0	2.5	0.5	0.3	6.4	6.2	13.4	2.1	1.0	2.0	0.6	1.4	1.3	1.4
PAW	GBRV12/ABINIT	0.9	0.8	1.0	1.0	0.8	0.9	4.0	1.3	1.3	1.1	1.9	2.0	0.8		4.1	1.5	1.6	1.5	1.1	2.0	1.1	2.3	1.0	0.9	0.7	0.8	0.7	2.8	1.0	0.7	6.4	6.3	15.1	2.5	1.5	2.4	1.1	1.8	1.7	1.8
	GPAW06/GPAW	3.8	3.8	3.8	3.8	3.8	3.5	3.1	3.4	3.5	3.4	3.2	2.6	3.8	4.1		3.6	3.5	3.2	3.5	3.0	3.8	2.8	3.7	3.8	4.0	3.8	4.0	5.6	3.9	3.6	7.4	7.6	12.3	4.5	3.0	3.0	3.6	3.7	3.8	3.7
	GPAW09/ABINIT	1.3	1.3	1.3	1.3	1.3	1.3	4.1	1.7	1.7	1.5	2.2	2.1	1.3	1.5	3.6		0.6	1.5	1.4	2.0	1.5	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	2.3	1.2	1.7	1.7	1.7
	GPAW09/GPAW	1.5	1.5	1.6	1.6	1.5	1.5	4.1	1.9	1.8	1.7	2.3	2.2	1.5	1.6	3.5	0.6		1.6	1.5	2.1	1.6	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	2.3	1.5	1.8	1.8	1.8
	JTH01/ABINIT	1.2	1.2	1.3	1.3	1.2	1.0	3.4	1.0	1.2	0.9	1.3	1.1	1.2	1.5	3.2	1.5	1.6		0.9	1.5	1.4	1.9	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	1.5	1.2	1.4	1.4	1.4
	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	1.1	3.5	1.4	1.5	0.9		1.4	0.9	1.9	0.7	0.7	1.2	1.2	1.2	2.6	0.7	0.6	6.3	6.2	13.4	2.2	1.2	1.9	0.7	1.4	1.4	1.4
	PSlib031/QE	1.6	1.6	1.7	1.7	1.6	1.5	3.3	1.5	1.4	1.6	1.8	1.6	1.6	2.0	3.0	2.0	2.1	1.5	1.4		1.6	1.5	1.6	1.6	2.0	1.9	2.0	3.1	1.6	1.5	6.1	5.8	12.8	2.4	1.6	1.7	1.5	2.1	2.2	2.1
	PSlib100/QE	0.9	0.8	1.0	1.0	0.8	0.8	3.9	1.3	1.3	1.1	1.8	1.8	0.8	1.1	3.8	1.5	1.6	1.4	0.9	1.6		1.7	1.0	0.8	1.1	1.2	1.2	2.2	0.9	0.7	6.1	5.9	13.5	2.1	1.4	1.9	0.9	1.6	1.6	1.6
	VASP2007/VASP	2.1	2.1	2.2	2.2	2.0	1.9	2.8	1.9	1.9	1.9	1.7	1.4	2.0	2.3	2.8	2.4	2.5	1.9	1.9	1.5	1.7		1.8	2.1	2.1	2.2	2.1	3.5	2.1	1.9	6.5	6.1	12.4	3.0	2.2	1.7	1.9	2.5	2.4	2.5
	VASP2012/VASP	0.7	0.6	0.8	0.8	0.6	0.7	3.9	1.2	1.2	1.0	1.8	1.9	0.7	1.0	3.7	1.4	1.6	1.4	0.7	1.6	1.0	1.8		0.7	1.1	1.2	1.1	2.5	0.8	0.6	6.5	6.3	13.4	2.2	1.2	2.1	0.9	1.6	1.5	1.6
	VASPGW2015/VASP	0.4	0.4	0.6	0.6	0.4	0.6	4.0	1.0	1.0	0.8	1.8	2.0	0.3	0.9	3.8	1.3	1.5	1.3	0.7	1.6	0.8	2.1	0.7		1.1	1.1	1.1	2.6	0.5	0.4	6.6	6.2	13.7	2.2	1.1	2.2	0.7	1.5	1.4	1.5
USPP	GBRV12/QE	1.1	1.0	1.1	1.1	0.9	1.0	4.0	1.3	1.4	1.2	1.9	2.0	0.9	0.7	4.0	1.6	1.7	1.5	1.2	2.0	1.1	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	2.1	1.2	1.6	1.5	1.6
	GBRV14/CASTEP	1.1	1.1	1.2	1.2	1.0	1.0	4.0	1.3	1.4	1.3	1.9	2.0	1.0	0.8	3.8	1.6	1.7	1.5	1.2	1.9	1.2	2.2	1.2	1.1	0.4		0.3	2.6	0.9	0.9	6.2	6.3	15.0	2.4	1.6	2.1	1.1	1.5	1.5	1.5
	GBRV14/QE	1.0	1.0	1.1	1.1	0.9	1.0	4.1	1.3	1.4	1.3	1.9	2.0	1.0	0.7	4.0	1.6	1.7	1.5	1.2	2.0	1.2	2.1	1.1	1.1	0.1	0.3		2.6	1.0	0.8	6.3	6.3	15.2	2.3	1.4	2.1	1.2	1.6	1.5	1.5
	OTFG7/CASTEP	2.5	2.5	2.6	2.6	2.5	2.6	5.8	3.1	2.9	3.0	3.8	3.8	2.5	2.8	5.6	2.5	2.7	3.0	2.6	3.1	2.2	3.5	2.5	2.6	2.6	2.6	2.6		2.2	2.4	4.8	5.7	14.5	2.7	2.9	3.4	2.4	2.6	2.6	2.6
	OTFG9/CASTEP	0.4	0.5	0.7	0.7	0.5	0.7	4.1	1.1	1.0	1.0	1.8	2.0	0.5	1.0	3.9	1.4	1.5	1.4	0.7	1.6	0.9	2.1	0.8	0.5	1.0	0.9	1.0	2.2		0.6	6.3	6.2	13.6	2.2	1.1	2.1	0.8	1.5	1.4	1.5
	SSSP/QE	0.4	0.3	0.6	0.6	0.3	0.5	3.9	1.0	0.9	0.8	1.6	1.7	0.3	0.7	3.6	1.3	1.4	1.1	0.6	1.5	0.7	1.9	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	1.4	1.2	1.3
	Vdb/CASTEP	6.4	6.4	6.4	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	6.5	6.5	6.6	6.3	6.2	6.3	4.8	6.3	6.4		9.6	16.3	6.6	6.1	6.6	6.4	5.7	5.8	5.7
	Vdb2/DACAPO	6.3	6.3	6.3	6.3	6.3	6.3	7.2	6.4	6.4	6.5	7.0	6.9	6.2	6.3	7.6	6.1	6.1	6.5	6.2	5.8	5.9	6.1	6.3	6.2	6.4	6.3	6.3	5.7	6.2	6.2	9.6		17.9	6.2	5.9	6.4	6.1	6.5	6.5	6.5
NCPP	FHI98pp/ABINIT	13.5	13.4	13.6	13.6	13.4	13.2	13.0	13.7	13.0	13.2	13.0	12.3	13.4	15.1	12.3	13.6	13.6	13.0	13.4	12.8	13.5	12.4	13.4	13.7	15.3	15.0	15.2	14.5	13.6	13.6	16.3	17.9		14.3	8.5	13.0	13.3	13.3	13.6	13.4
	HGH/ABINIT	2.2	2.2	2.2	2.2	2.2	2.0	4.9	2.4	2.3	2.2	2.8	2.8	2.1	2.5	4.5	2.3	2.5	2.2	2.2	2.4	2.1	3.0	2.2	2.2	2.3	2.4	2.3	2.7	2.2	2.1	6.6	6.2	14.3		0.9	2.6	2.0	2.0	2.0	2.0
	HGH-NLCC/BigDFT	1.1	1.1	1.2	1.2	1.1	1.0	3.6	1.2	1.2	1.1	1.7	1.6	1.0	1.5	3.0	1.7	1.8	1.3	1.2	1.6	1.4	2.2	1.2	1.1	1.4	1.6	1.4	2.9	1.1	1.0	6.1	5.9	8.5	0.9		1.8	1.1	1.5	1.4	1.4
	MBK2013/OpenMX	2.1	2.1	2.0	2.0	2.1	1.9	3.2	1.8	1.8	1.8	1.9	1.5	2.0	2.4	3.0	2.3	2.3	1.5	1.9	1.7	1.9	1.7	2.1	2.2	2.1	2.1	2.1	3.4	2.1	2.0	6.6	6.4	13.0	2.6	1.8		2.0	2.2	2.2	2.2
	ONCVPSP(PD0.1)/ABINIT	0.7	0.7	0.8	0.8	0.7	0.6	3.7	1.0	1.0	0.8	1.6	1.7	0.6	1.1	3.6	1.2	1.5	1.2	0.7	1.5	0.9	1.9	0.9	0.7	1.2	1.1	1.2	2.4	0.8	0.7	6.4	6.1	13.3	2.0	1.1	2.0		1.3	1.4	1.3
	ONCVPSP(SG15)1/CASTEP	1.5	1.4	1.5	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	1.4	2.1	1.6	2.5	1.6	1.5	1.6	1.5	1.6	2.6	1.5	1.4	5.7	6.5	13.3	2.0	1.5	2.2	1.3		0.3	0.1
	ONCVPSP(SG15)1/QE	1.4	1.3	1.4	1.4	1.3	1.3	4.1	1.6	1.6	1.5	2.1	1.9	1.3	1.7	3.8	1.7	1.8	1.4	1.4	2.2	1.6	2.4	1.5	1.4	1.5	1.5	1.5	2.6	1.4	1.2	5.8	6.5	13.6	2.0	1.4	2.2	1.4	0.3		0.3
	ONCVPSP(SG15)2/CASTEP	1.4	1.4	1.5	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	1.4	2.1	1.6	2.5	1.6	1.5	1.6	1.5	1.5	2.6	1.5	1.3	5.7	6.5	13.4	2.0	1.4	2.2	1.3	0.1	0.3	

DFT codes using PAW

- VASP license
- Abinit free
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Importance of good **potential database**

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