

# **Pseudopotentials**

## **Theory and application**

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# What is a pseudopotential?

The fundamental idea of a “pseudopotential” is the replacement of one problem with another:

- A difficult problem with one that is easier to solve
- And which leads to the same result for certain properties

What is the problem we deal with in electronic structure?

- The potential due to the nuclei is so strong that the lowest energy states are strongly bound near the nucleus
- These “core states” are filled and are almost inert. They hardly change when atoms bind together to form a solid
- The higher energy “valence states” extend to larger distances from the nuclei. These are the states that determine the properties of the solid:
  - Binding energy
  - Crystal structure
  - Whether it is a metal or insulator
  - .....

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# The goal for a pseudopotential in a solid

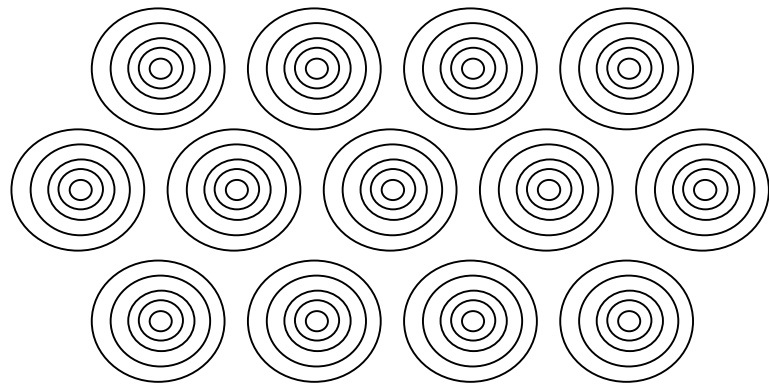
The goal for a pseudopotential in a solid is to replace the problem with a strong potential with a weaker potential:

- That has the same properties for the valence states
  - The same crystal structure
  - The same band structure for the valence bands
  - .....

We want the same properties without having to deal with the strongly bound core states!

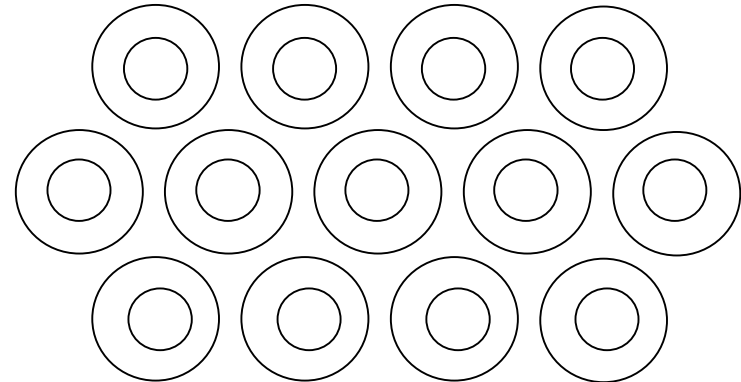
# The goal for a pseudopotential in a solid

To replace this problem



Strong potential with  
core and valence  
states

With this problem



Weak potential with  
no core states and  
only valence states

# Remember Shobhana's analogy

- “Dummy cops” used by many law-enforcement agencies!

Stick a mannequin in uniform by the highway ... if it looks like a cop, it works like a cop!

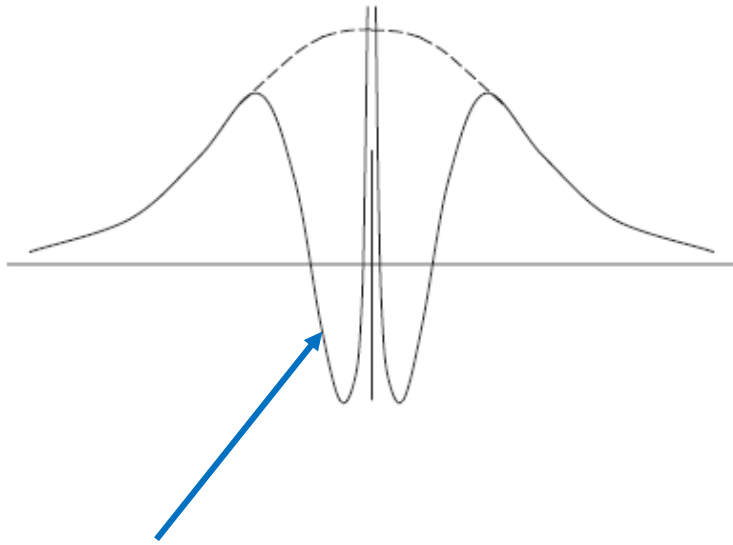
Don't care about internal structure as long as it works right!

But cheaper!!

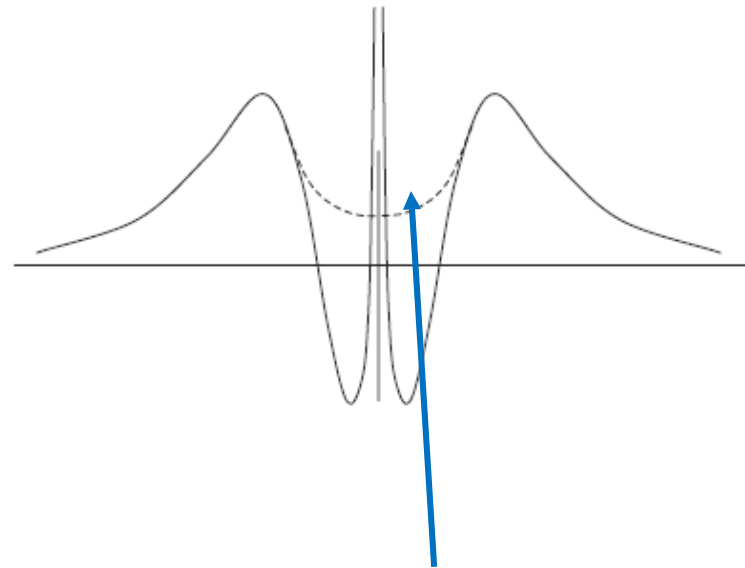
Obviously it can't reproduce all the functions of a real cop, but **should be convincing enough** to produce desired results....



# Pseudofunctions



Valence state that is  
orthogonal to the core states



Smooth pseudofunction that  
has the same properties  
outside the core region

# Method that is very useful for valence states in a crystal: Plane Waves

The good thing about PWs

They are general

Not biased to assume some atomic-like form

The bad thing about PWs

They are general

Requires very many PWs to reconstruct the atomic-like aspects of actual wavefunctions

Advantages of PWs

Simple algorithms – fast FFTs

Can be very efficient even for many PWs

So simple and efficient that they have made it possible develop many new methods – MD, response functions, ...

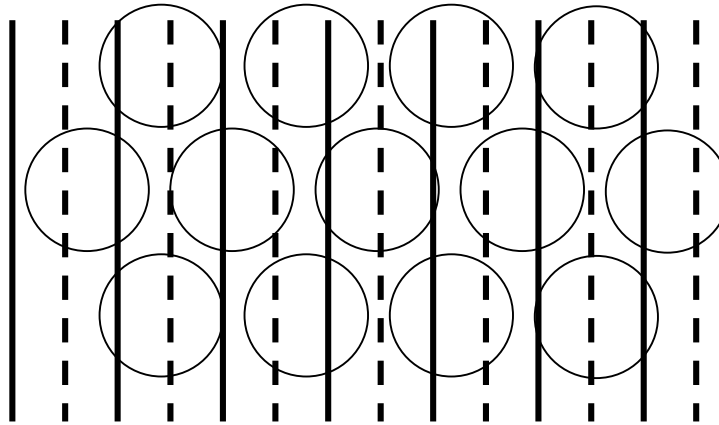
Relation to other methods

Many PW methods – APW, PAW, pseudopotential -- can be related by the effect of the core region upon to wavefunctions outside the core (phase shifts)



# Plane Waves

- A general approach with many advantages



- Kohn-Sham  
Equations  
in a crystal

$$\psi_{i,\mathbf{k}}(\mathbf{r}) \propto \sum_m c_{i,m}(\mathbf{k}) \times \exp(i(\mathbf{k} + \mathbf{G}_m) \cdot \mathbf{r}) \quad (1)$$

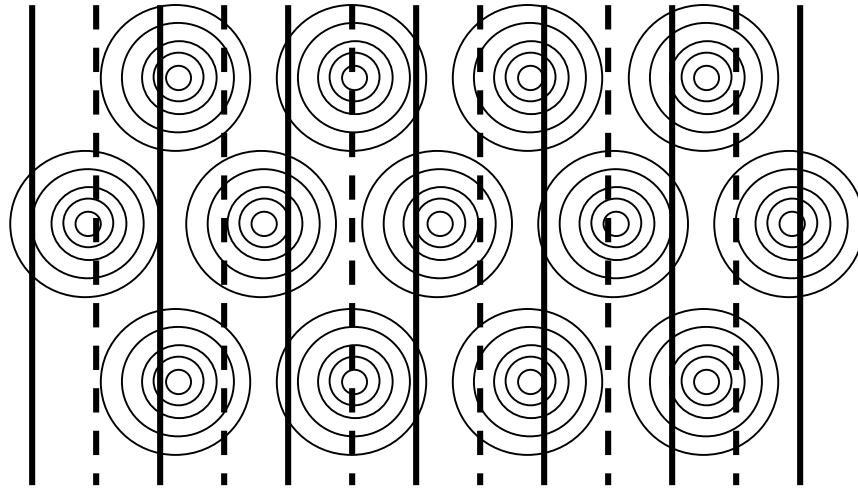
$$\sum_{m'} H_{m,m'}(\mathbf{k}) c_{i,m'}(\mathbf{k}) = \varepsilon_i(\mathbf{k}) c_{i,m}(\mathbf{k}) \quad (2)$$

$$H_{m,m'}(\mathbf{k}) = \frac{\hbar^2}{2m_e} |\mathbf{k} + \mathbf{G}_m|^2 \delta_{m,m'} + V_{eff}(\mathbf{G}_m - \mathbf{G}_{m'}). \quad (3)$$

- *The problem is the atoms! High Fourier components!*

# Why not use plane waves directly?

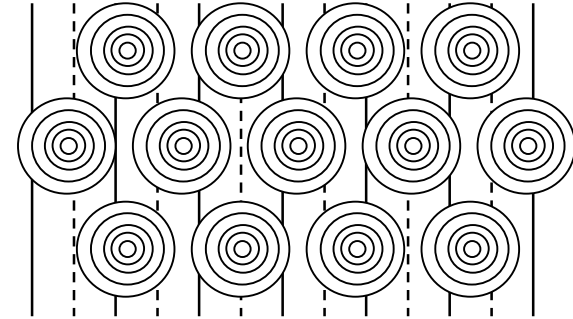
- Basic problem - many electrons in the presence of the nuclei



- Core states – strongly bound to nuclei – atomic-like
- Valence states – change in the material – determine the bonding, electronic and optical properties, magnetism, .....

# Basic Methods with Plane Waves

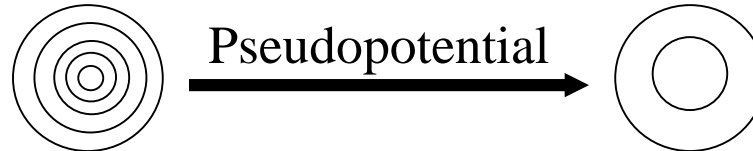
- Pseudopotentials (PPs)
  - Replace cores by smooth pseudopotentials
  - Then use Fourier Expansions directly
  - The speed of Fast Fourier Transforms
- Ultrasoft and a type of Augmentation (PAW)
  - Add localized functions around the atoms in addition to the plane waves
  - Can consider as a combination of the ideas from pseudopotentials and APW
- Original Augmentation method (APW)
  - Define spheres around atoms
  - Solve with plane waves outside, spherical harmonics inside
  - Most general form – (L)APW - linearization very important for simplifying calculations



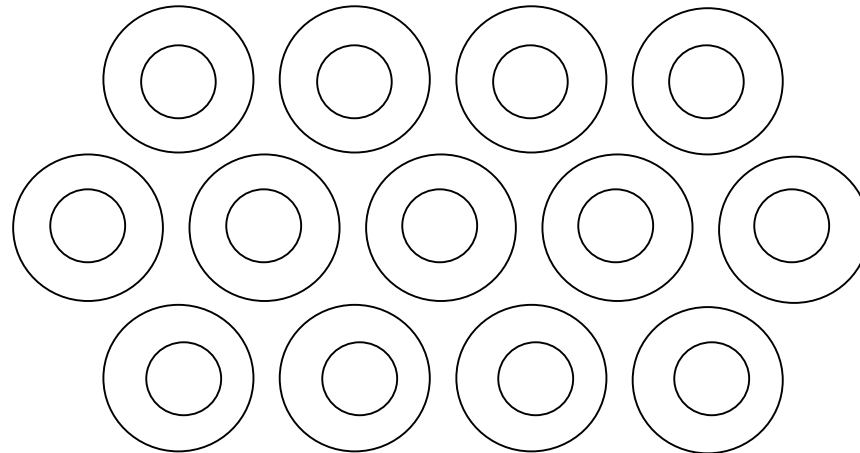
# Pseudopotentials

- **Pseudopotential Method** – replace each potential

1 atom



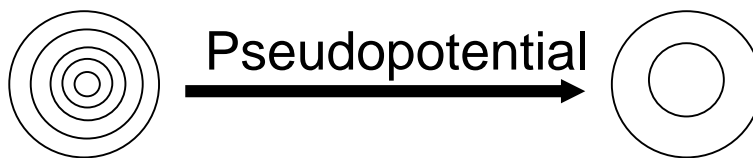
2 solid



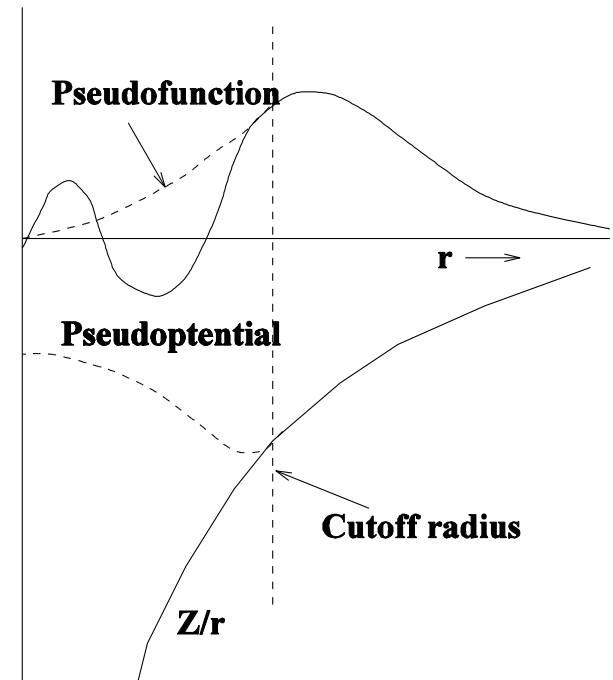
- 1 Generate **Pseudopotential** in atom (spherical)
- 2 Use **Pseudopotential** in the solid

# Norm-Conserving Pseudopotentials

- Norm-Conserving Pseudopotential (NCPP)
  - Hamann, Schluter, Chiang (1979)

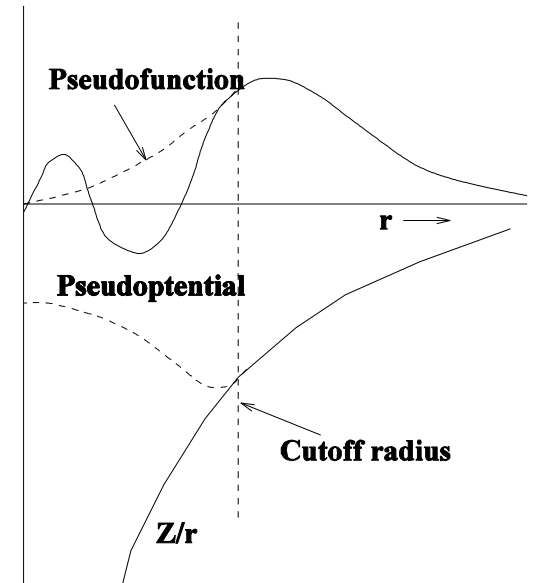


- Generate weak pseudopotential in atom with same properties for valence states as the strong all-electron potential
- Conditions
  - Potential same for  $r > R_c$
  - Pseudofunction “norm-conserving” for  $r < R_c$



# Norm-Conserving Pseudopotentials

- Summary of the theory and steps in constructing a NCPP
- 1. DFT calculations for the all-electron atom – find the valence eigenvalues and eigenfunctions for each angular momentum  $L$
- 2. Construct a pseudofunction that is the same outside  $R_c$  and is continued inside smoothly
- 3. Require “norm conservation” which means the function is normalized. This is satisfied if the integral over the core region is the same as for the original valence function.
- 4. Find the pseudopotential by inverting the Schrodinger equation:  
$$V(r) \psi(r) = e\psi(r) + (\hbar^2/2m) [(2/r) (d\psi/dr) + (d^2\psi/dr^2)]$$
  
Done separately for each ang. mom.  $L$

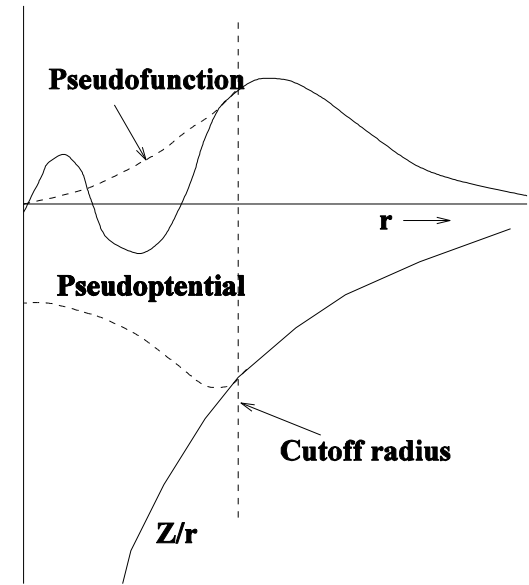


# Norm-Conserving Pseudopotentials

- Summary of the properties of a NCPP

- Properties of a NCPP

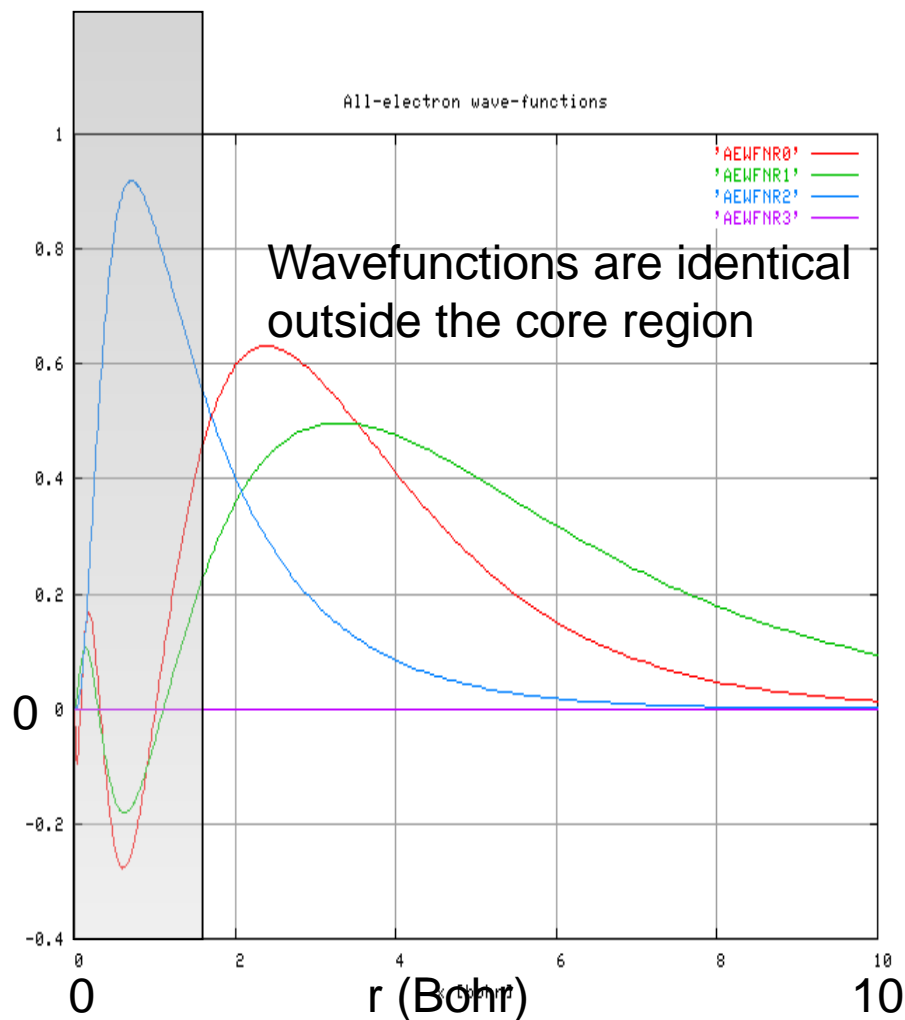
- The potential is “non-local” – it is not simply a function of position – the potential for each angular momentum is different
- An elegant proof shows that if the pseudopotential is norm-conserving, then it also has the property that the logarithmic derivative is not only correct at the given energy  $e$ , but also correct to linear order for energies  $\varepsilon + \Delta\varepsilon$
- The last point is the feature that makes the potentials more “transferable” from the atom to the molecule or solid where the energies change.



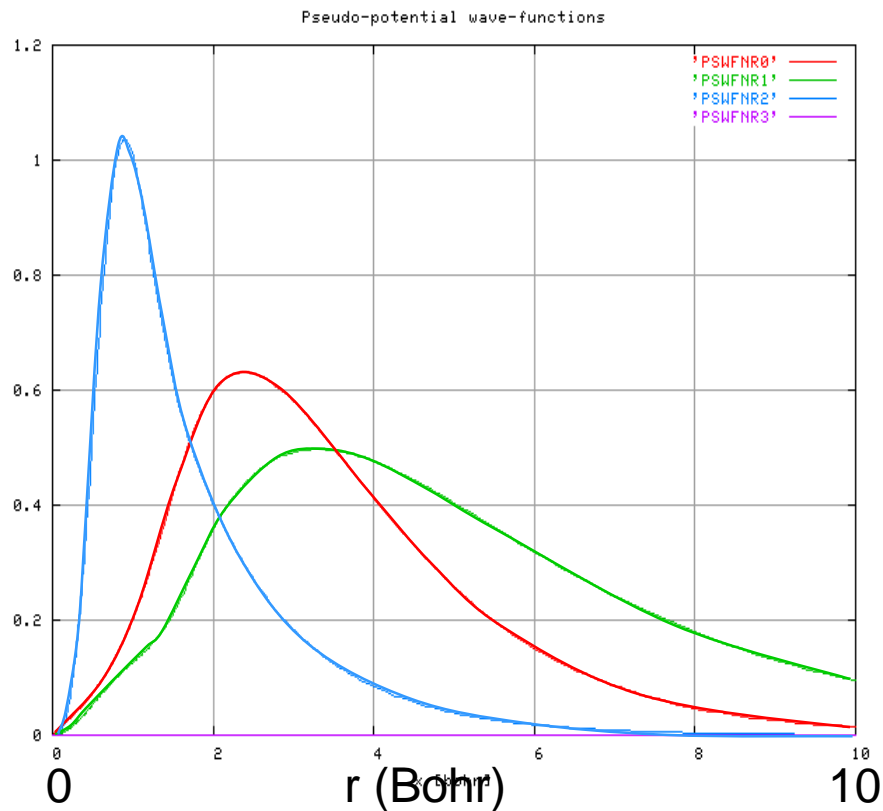
**Nonlocal - Different  $V_l(r)$   
for different angular  
momenta  $l$**

# Example -Fe – s,p,d valence wavefunctions – $r \psi(r)$

## All electron functions



## Pseudo functions

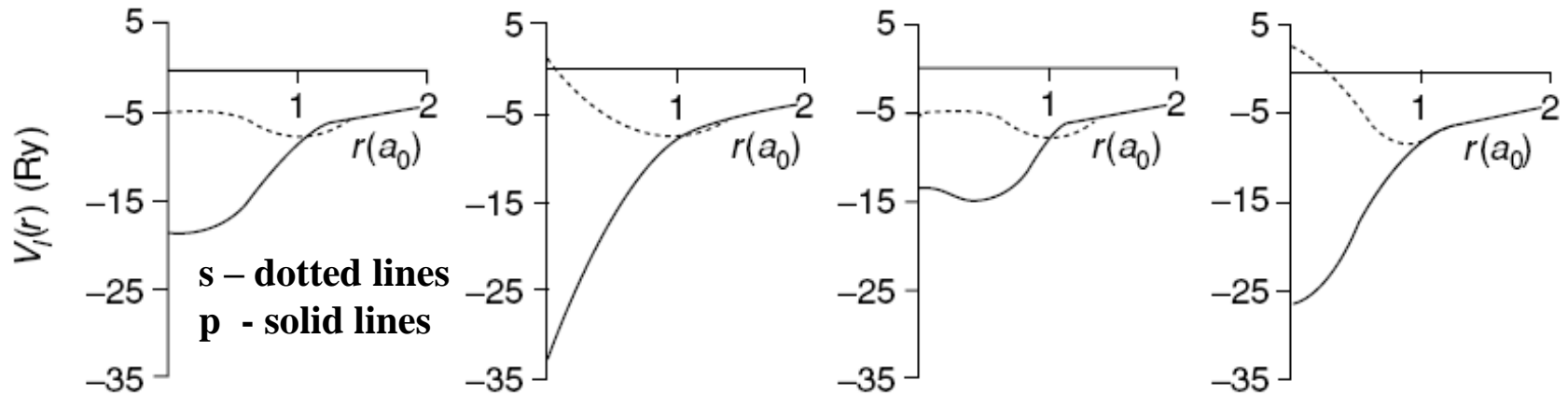


From <http://www.tddft.org/>



# Examples of pseudopotentials

**All these pseudopotentials give essentially the same results in a calculation on a solid carbon!**



**Figure 11.5 in the book**

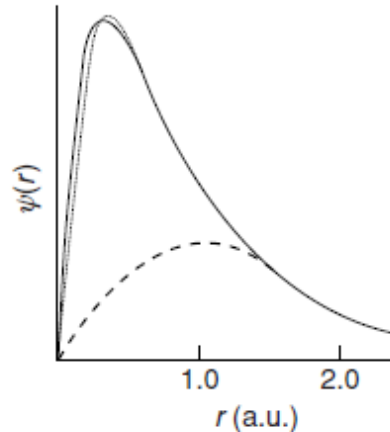
## Key points:

The potentials are “non-local” – different for different angular momenta. A complication but it can be done by projecting plane waves onto spherical harmonics

Many different potentials can give the same wavefunctions outside the core region – and essentially the same results in a solid

# Ultrasoft pseudopotentials

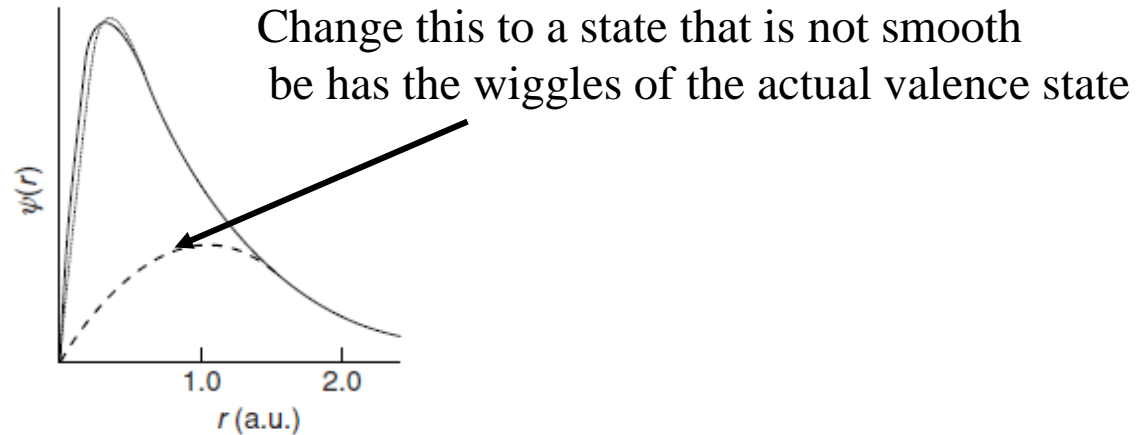
- Forerunner for PAW – next slide



- Smooth functions extend throughout crystal – expressed in plane waves - like norm-conserving pseudopotentials
- Add functions inside the core region to better represent pseudofunctions – Very helpful for O, transition metals, . . . .
- Equations for smooth functions similar to norm-conserving pseudopotential Eqs. – but generalized eigenvalue problem
- Can use FFTs as in norm-conserving pseudopotentials

# Projector Augmented Plane Wave (PAW)

- PAW – add core functions in core region



- Smooth functions extend throughout crystal – expressed in plane waves - like ultrasoft pseudopotentials
- Add core functions in core regions – in the simplest form the functions are assumed to be the same as in an atom
- Equations for smooth functions similar to ultrasoft PP Eqs. while having a full atomic like functions inside sphere
- Can use FFTs as in pseudopotentials

# Kleinman-Bylander separable potential

- Norm-conserving potentials are:
  - Different radial dependence for each angular momentum -- semilocal
- This can be transformed into a separable operator

$$\hat{V}_{\text{NL}} = V_{\text{local}}(r) + \sum_{lm} \frac{|\psi_{lm}^{\text{PS}} \delta V_l\rangle \langle \delta V_l \psi_{lm}^{\text{PS}}|}{\langle \psi_{lm}^{\text{PS}} | \delta V_l | \psi_{lm}^{\text{PS}} \rangle},$$

# Results agree with experiment (in important classes of materials)

Different methods agree  
(when done carefully)

Method	C		Si		CaF <sub>2</sub>		bcc Fe		
	<i>a</i>	<i>B</i>	<i>a</i>	<i>B</i>	<i>a</i>	<i>B</i>	<i>a</i>	<i>B</i>	<i>m</i>
NCP <sup>a</sup>	3.54	460	5.39	98	5.21	90	2.75 <sup>c</sup>	226 <sup>c</sup>	
PAW <sup>a</sup>	3.54	460	5.38	98	5.34	100			
PAW <sup>b</sup>	3.54	460	5.40	95	5.34	101	2.75	247	2.00
USPP <sup>b</sup>	3.54	461	5.40	95	5.34	101	2.72	237	2.08
LAPW <sup>a</sup>	3.54	470	5.41	98	5.33	110	2.72 <sup>d</sup>	245 <sup>d</sup>	2.04 <sup>d</sup>
EXP <sup>a</sup>	3.56	443	5.43	99	5.45	85-90	2.87 <sup>d</sup>	172 <sup>d</sup>	2.12 <sup>d</sup>

- **a** – lattice constant, **B** – bulk modulus, **m** – magnetization

- <sup>a</sup>Holzwarth, *et al.*; <sup>b</sup>Kresse & Joubert; <sup>c</sup>Cho & Scheffler; <sup>d</sup>Stizrude, *et al.*

# Comparison of Methods for DFT

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## RESEARCH ARTICLE SUMMARY

### DFT METHODS

## Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere,\* Gustav Bihlmayer, Torbjörn Björkman, Peter Blaha, Stefan Blügel, Volker Blum, Damien Caliste, Ivano E. Castelli, Stewart J. Clark, Andrea Dal Corso, Stefano de Gironcoli, Thierry Deutsch, John Kay Dewhurst, Igor Di Marco, Claudia Draxl, Marcin Dułak, Olle Eriksson, José A. Flores-Livas, Kevin F. Garrity, Luigi Genovese, Paolo Giannozzi, Matteo Giantomassi, Stefan Goedecker, Xavier Gonze, Oscar Grånäs, E. K. U. Gross, Andris Gulans, François Gygi, D. R. Hamann, Phil J. Hasnip, N. A. W. Holzwarth, Diana Iușan, Dominik B. Jochym, François Jollet, Daniel Jones, Georg Kresse, Klaus Koepernik, Emine Küçükbenli, Yaroslav O. Kvashnin, Inka L. M. Locht, Sven Lubeck, Martijn Marsman, Nicola Marzari, Ulrike Nitzsche, Lars Nordström, Taisuke Ozaki, Lorenzo Paulatto, Chris J. Pickard, Ward Poelmans, Matt I. J. Probert, Keith Refson, Manuel Richter, Gian-Marco Rignanese, Santanu Saha, Matthias Scheffler, Martin Schlipf, Karlheinz Schwarz, Sangeeta Sharma, Francesca Tavazza, Patrik Thunström, Alexandre Tkatchenko, Marc Torrent, David Vanderbilt, Michiel J. van Setten, Veronique Van Speybroeck, John M. Wills, Jonathan R. Yates, Guo-Xu Zhang, Stefaan Cottenier\*

**The main conclusion: Methods agree when done carefully**

**Science 25 march 2018**

# Comparison of Methods for DFT

		AE												PAW										USPP					NCPP											
	Rk	exciting	FHI-aims/tight	FHI-aims/really_tight	FLMUR	FPLO/default	FPLO/T+P	FPLO/T+P+q	RSPT	WIEN2k/default	WIEN2k/enhanced	WIEN2k/acc	GBRV12/ABINIT	CPAW06/CPAW	CPAW09/ABINIT	CPAW09/CPAW	JTB01/ABINIT	JTB02/ABINIT	PSlib031/QE	PSlib100/QE	VASP2007/VASP	VASP2012/VASP	VASPO62015/VASP	GBRV12/QE	GBRV14/CASTEP	GBRV14/QE	OTFG/CASTEP	OTFG9/CASTEP	SSRP/QE	Vdb/CASTEP	Vdb2/DACAP0	FHI98pp/ABINIT	BGR/ABINIT	BGR-MLCC/BigDFT	MUK2013/QepoMK	ONCVPSPP (P0.1)/ABINIT	ONCVPSPP (SG15.1)/CASTEP	ONCVPSPP (SG15.1)/QE	ONCVPSPP (SG15.12)/CASTEP	
AE	Rk	03	06	06	03	06	29	10	10	05	17	18	03	05	38	13	15	12	06	16	05	21	07	04	11	11	10	25	04	04	64	63	135	22	11	21	07	15	14	14
	exciting	03	05	05	01	05	29	10	09	08	17	18	02	08	38	13	15	12	06	16	08	21	06	04	10	11	10	25	05	03	64	63	134	22	11	21	07	14	13	14
	FHI-aims/tight	06	05	00	05	07	38	09	11	07	18	18	05	10	38	13	16	13	07	17	10	22	08	06	11	12	11	26	07	06	64	63	136	22	12	20	08	15	14	15
	FHI-aims/really_tight	06	05	00	05	07	38	09	11	08	18	18	05	10	38	13	16	13	07	17	10	22	08	06	11	12	11	26	07	06	65	63	136	22	12	20	08	15	14	15
	FHI-aims/tier2	03	01	05	05	05	39	09	09	08	17	18	02	08	38	13	15	12	06	16	08	20	06	04	09	10	09	25	05	03	64	63	134	22	11	21	07	14	13	14
	FLMUR	06	05	07	07	05	36	08	08	06	14	15	04	05	35	13	15	10	06	15	08	19	07	06	10	10	10	26	07	05	65	63	132	20	10	15	06	13	13	13
	FPLO/default	29	29	28	28	29	26	31	26	33	29	25	39	40	31	41	41	24	26	33	39	28	39	40	40	40	41	58	41	39	79	72	130	49	26	32	37	41	41	
	FPLO/T+P	10	10	09	09	09	08	31	08	07	14	14	09	13	24	17	19	10	09	15	13	19	12	10	13	13	13	31	11	10	66	64	137	24	12	18	10	16	16	16
	FPLO/T+P+q	10	05	11	11	05	08	36	08	05	15	15	09	13	25	17	18	12	09	14	13	19	12	10	14	14	14	29	10	09	64	64	130	23	12	18	10	16	16	16
	RSPT	05	08	07	08	08	06	33	07	05	13	13	08	11	24	15	17	09	07	16	11	19	10	08	12	13	13	30	10	08	67	65	132	22	11	18	08	15	15	15
	WIEN2k/default	17	17	18	18	17	14	29	14	15	13	09	17	19	32	22	23	13	15	18	18	17	18	18	19	19	19	38	18	16	71	70	130	28	17	15	16	21	21	21
WIEN2k/enhanced	18	18	18	18	18	15	25	14	15	13	09	18	20	26	21	22	11	15	16	18	14	19	20	20	20	20	38	20	17	69	69	123	28	16	15	17	19	19	19	
WIEN2k/acc	03	02	05	05	02	04	39	09	09	08	17	18	08	38	13	15	12	05	16	08	20	07	03	09	10	10	25	05	03	64	62	134	21	10	20	06	14	13	14	
PAW	GBRV12/ABINIT	09	08	10	10	08	09	40	13	13	11	15	20	08	41	15	16	15	11	20	11	23	10	09	07	08	07	28	10	07	64	63	151	25	15	24	11	18	17	18
	CPAW06/CPAW	38	38	38	38	38	35	31	34	35	34	32	26	38	41	36	25	22	35	30	38	28	27	38	40	38	40	56	29	36	74	76	123	45	30	30	26	37	38	37
	CPAW09/ABINIT	13	13	13	13	13	41	17	17	15	22	21	13	15	36	06	15	14	20	15	24	14	13	16	16	16	25	14	13	65	61	136	23	17	23	12	17	17	17	
	CPAW09/CPAW	15	15	16	16	15	15	41	19	18	17	23	22	15	16	35	06	16	15	21	16	25	16	15	17	17	17	27	15	14	65	61	136	25	18	23	15	18	18	18
	JTB01/ABINIT	12	12	13	13	12	10	34	10	12	09	13	11	12	15	32	15	16	09	15	14	19	14	13	15	15	15	30	14	11	65	65	130	22	13	15	12	14	14	14
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	VASP2007/VASP	21	21	22	22	20	19	28	19	19	17	14	20	23	28	24	25	19	19	15	17	18	21	21	22	21	22	35	21	19	65	61	124	30	22	17	15	25	24	25
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	VASPO62015/VASP	04	04	06	06	04	06	40	10	10	08	18	20	03	09	38	13	15	13	07	16	08	21	07	11	11	11	26	05	04	66	62	137	22	11	22	07	15	14	15
USPP	GBRV12/QE	11	10	11	11	09	10	40	13	14	12	19	20	09	40	16	17	15	12	20	11	21	11	11	04	01	26	10	08	63	64	153	23	14	21	12	16	15	16	
	GBRV14/CASTEP	11	11	12	12	10	10	40	13	14	13	19	20	10	40	16	17	15	12	19	12	22	12	11	04	03	26	09	09	62	63	150	24	16	21	11	15	15	15	
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	OTFG/CASTEP	25	25	26	26	25	26	58	31	29	30	38	38	25	28	56	25	27	30	26	31	22	35	25	26	26	26	26	22	24	48	57	145	27	29	34	24	26	26	26
	OTFG9/CASTEP	04	05	07	07	05	07	41	11	10	10	18	20	05	10	39	14	15	14	07	16	09	21	08	05	10	09	10	22	06	63	62	136	22	11	21	08	15	14	15
	SSRP/QE	04	03	06	06	03	05	39	10	09	08	16	17	03	07	26	13	14	11	06	15	07	19	06	04	08	09	08	24	06	64	62	136	21	10	20	07	14	12	13
	Vdb/CASTEP	64	64	64	65	64	65	79	66	64	67	71	69	64	74	65	65	65	63	61	61	65	65	66	63	62	63	48	63	64	96	163	66	61	66	64	57	58	57	
	Vdb2/DACAP0	63	63	63	63	63	63	72	64	64	65	70	69	62	63	76	61	61	65	62	58	59	61	62	62	64	63	57	62	96	179	62	59	64	61	65	65	65		
	FHI98pp/ABINIT	135	134	136	136	134	132	130	137	130	132	130	123	134	151	123	136	136	130	134	128	135	124	134	137	153	150	152	145	136	136	163	179	143	85	130	133	133	136	134
	BGR/ABINIT	22	22	22	22	22	20	49	24	23	22	28	28	21	25	45	23	25	22	22	24	21	30	22	22	23	24	23	27	22	21	66	62	143	09	26	20	20	20	20
BGR-MLCC/BigDFT	11	11	12	12	11	10	36	12	12	11	17	16	10	15	30	17	18	13	12	16	14	22	12	11	14	16	14	29	11	10	61	59	85	09	18	11	15	14	14	
MUK2013/QepoMK	21	21	20	20	21	19	32	18	18	18	19	15	20	24	30	23	23	15	19	17	17	21	22	21	21	21	34	21	20	66	64	130	26	18	20	22	22	22		
NCPP	ONCVPSPP (P0.1)/ABINIT	07	07	08	08	07	06	37	10	10	08	16	17	06	11	26	12	15	12	07	15	09	09	07	12	11	12	24	08	07	64	61	133	20	11	20	13	14	13	
	ONCVPSPP (SG15.1)/CASTEP	15	14	15	15	14	13	41	16	16	15	21	19	14	18	37	17	18	14	14	21	16	25	16	15	16	15	16	26	15	14	57	65	133	20	15	22	13	03	01
	ONCVPSPP (SG15.1)/QE	14	13	14	14	13	13	41	16	16	15	21	19	13	17	38	17	18	14	14	22	16	24	15	14	15	15	15	26	14	12	58	65	136	20	14	22	14	03	03
	ONCVPSPP (SG15.2)/CASTEP	14																																						

# Comparison of Methods

The main conclusion:  
Modern methods done carefully agree

		average $\langle \Delta \rangle$	AE						
			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	
PAW	GBRV12/ABINIT	0.9	0.9	0.8	0.8	0.9	1.3	1.1	0.8
	GPAW09/ABINIT	1.4	1.3	1.3	1.3	1.3	1.7	1.5	1.3
	GPAW09/GPAW	1.6	1.5	1.5	1.5	1.5	1.8	1.7	1.5
	JTH02/ABINIT	0.6	0.6	0.6	0.6	0.6	0.9	0.7	0.5
	PSlib100/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
USPP	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
	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/DACAP0	6.3	6.3	6.3	6.3	6.3	6.4	6.5	6.2
NCPP	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
	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
	ONCVSP (PD0.1)/ABINIT	0.7	0.7	0.7	0.7	0.6	1.0	0.8	0.6
	ONCVSP (SG15)1/QE	1.4	1.4	1.3	1.3	1.3	1.6	1.5	1.3
	ONCVSP (SG15)2/CASTEP	1.4	1.4	1.4	1.4	1.3	1.6	1.5	1.4



# Pseudopotentials

		AE						
		average $\langle \Delta \rangle$	Elk	exciting	FHI-aims/tier2	FLEUR	FPLM/T+T+s	RSPT
AE	Elk	0.6		0.3	0.3	0.6	1.0	0.9
	exciting	0.5	0.3		0.1	0.5	0.9	0.8
	FHI-aims/tier2	0.5	0.3	0.1		0.5	0.9	0.8
	FLEUR	0.6	0.6	0.5	0.5		0.8	0.6
	FPLM/T+T+s	0.9	1.0	0.9	0.9	0.8		0.9
	RSPT	0.8	0.9	0.8	0.8	0.6	0.9	
	WIEN2k/acc	0.5	0.3	0.2	0.2	0.4	0.9	0.8
PAW	GBRV12/ABINIT	0.9	0.9	0.8	0.8	0.9	1.3	1.1
	GPAW09/ABINIT	1.4	1.3	1.3	1.3	1.3	1.7	1.5
	GPAW09/GPAW	1.6	1.5	1.5	1.5	1.5	1.8	1.7
	JTH02/ABINIT	0.6	0.6	0.6	0.6	0.6	0.9	0.7
	PSlib100/QE	0.9	0.9	0.8	0.8	0.8	1.3	1.1
	VASPGW2015/VASP	0.6	0.4	0.4	0.4	0.6	1.0	0.8

USPP								
	GBRV14/CASTEP	1.1	1.1	1.1	1.0	1.0	1.4	1.3
	GBRV14/QE	1.1	1.0	1.0	0.9	1.0	1.4	1.3
	OTFG9/CASTEP	0.7	0.4	0.5	0.5	0.7	1.0	1.0
	SSSP/QE	0.5	0.4	0.3	0.3	0.5	0.9	0.8
	Vdb2/DACAPO	6.3	6.3	6.3	6.3	6.3	6.4	6.5
NCPP	FHI98pp/ABINIT	13.3	13.5	13.4	13.4	13.2	13.0	13.2
	HGH/ABINIT	2.2	2.2	2.2	2.2	2.0	2.3	2.2
	HGH-NLCC/BigDFT	1.1	1.1	1.1	1.1	1.0	1.2	1.1
	MBK2013/OpenMX	2.0	2.1	2.1	2.1	1.9	1.8	1.8
	ONCVSP (PD0.1)/ABINIT	0.7	0.7	0.7	0.7	0.6	1.0	0.8
	ONCVSP (SG15) 1/QE	1.4	1.4	1.3	1.3	1.3	1.6	1.5
	ONCVSP (SG15) 2/CASTEP	1.4	1.4	1.4	1.4	1.3	1.6	1.5

# Comparison of Methods for DFT

## One of the examples using QE

**Table S41.2. ONCVSPSP (SG15) 1/QE calculation settings and results per element.** Valence  $Z_{val}$ , k-point mesh in the full 1st Brillouin zone of the conventional cell  $kpts$  and number of irreducible k-points  $\#k$ , equilibrium volume per atom  $V_0$ , bulk modulus  $B_0$ , pressure derivative of the bulk modulus  $B_1$ .

	$Z_{val}$ [-]	kpts [-]	# k [-]	$V_0$ [ $\text{\AA}^3/\text{atom}$ ]	$B_0$ [GPa]	$B_1$ [-]
H	1	$28 \times 28 \times 20$	6 020	17.356	10.288	2.666
He	2	$40 \times 40 \times 22$	4 620	17.708	0.882	6.528
Li	3	$38 \times 38 \times 38$	27 436	20.244	13.846	3.345
Be	4	$52 \times 52 \times 28$	9 828	7.931	123.706	3.308
B	3	$26 \times 26 \times 24$	12 324	7.18	235.366	3.428
C	4	$48 \times 48 \times 12$	10 512	11.586	207.537	3.728
N	5	$16 \times 16 \times 16$	688	28.773	53.217	3.662
O	6	$26 \times 24 \times 24$	7 488	18.594	50.245	3.779
F	7	$16 \times 28 \times 14$	3 136	19.284	33.755	4.001
Ne	8	$22 \times 22 \times 22$	286	24.259	1.352	7.255
Na	9	$32 \times 32 \times 32$	16 384	37.113	7.762	3.697
Mg	10	$36 \times 36 \times 20$	9 900	22.961	36.548	4.05
Al	11	$24 \times 24 \times 24$	364	16.528	77.801	4.976
Si	4	$32 \times 32 \times 32$	8 448	20.522	87.495	4.268
-		$\blacksquare-\blacksquare\blacksquare-\blacksquare-\blacksquare-\blacksquare\blacksquare\blacksquare\blacksquare-\blacksquare-\blacksquare-\blacksquare$		---	----	-----
Au	19	$24 \times 24 \times 24$	364	17.982	138.715	6.007
Hg	20	$24 \times 24 \times 28$	1 092	29.55	7.772	9.92
Tl	13	$32 \times 32 \times 18$	7 056	31.361	26.88	5.448
Pb	14	$20 \times 20 \times 20$	220	31.943	40.077	5.575
Bi	15	$26 \times 26 \times 8$	4 108	36.917	42.82	4.69
Po	N/A	N/A	N/A	N/A	N/A	N/A
Rn	N/A	N/A	N/A	N/A	N/A	N/A

name and version of the code: QUANTUM ESPRESSO 5.1 (84)  
type of basis set: plane waves  
method: norm-conserving pseudopotentials (Schlipf-Gygi ONCVSP 2015-01-24 (94),

```
wave function cutoff      100 Ry
density cutoff           400 Ry
```

# Choice of pseudopotential?

What potential do you really want to use for a particular problem?

The best best potentials with huge numbers of plane waves?

Another choice that is less expensive

Now we arrive at reality!

What is good enough?

How do I verify that it is a good choicd?

.....

Discussion

# Following Slides from Shobhana on Pseudopotentials for QE

# Pseudopotentials



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- [Pseudo DoJo](#)
- [SG15 ONCV Potentials](#)
- [PSlibrary table](#)
- [Original QE PP table](#)
- [Hartwigesen-Goedecker-Hutter PP table](#)
- [Old FHI PP table](#)

<https://www.quantum-espresso.org/pseudopotentials>

# Quantum Espresso

 C.psp8.qz

# Pseudopotentials for Quantum Espresso - 2

- Click on element for which pseudopotential wanted.

ANY PP LIBRARY		OTHER OPTIONS	
1			2
H			He
3	4		
Li	Be		
5	6	7	8
B	C	N	O
9	10		
F	Ne		
11	12		
Na	Mg		
13	14	15	16
Al	Si	P	S
17	18		
Cl	Ar		
19	20		
K	Ca		
21	22	23	24
Sc	Ti	V	Cr
25	26	27	28
Mn	Fe	Co	Ni
29	30		
Cu	Zn		
31	32	33	34
Ga	Ge	As	Se
35	36		
Br	Kr		
37	38		
Rb	Sr		
39	40	41	42
Y	Zr	Nb	Mo
43	44	45	46
Tc	Ru	Rh	Pd
47	48	49	50
Ag	Cd	In	Sn
51	52	53	54
Sb	Te	I	Xe
55	56	57-70	
Cs	Ba		
71	72	73	74
Lu	Hf	Ta	W
75	76	77	78
Re	Os	Ir	Pt
79	80	81	82
Au	Hg	Tl	Pb
83	84	85	86
Bi	Po	At	Rn
87	88	89-102	
Fr	Ra		
103	104	105	106
Lr	Rf	Db	Sg
107	108	109	
Bh	Hs	Mt	
Lanthanoids		57	58
		La	Ce
		Pr	Nd
		Pm	Sm
		Eu	Gd
		Tb	Dy
		Ho	Er
		Tm	Yb
Actinoids		89	90
		Ac	Th
		Pa	U
		Np	Pu
		Am	Cm
		Bk	Cf
		Es	Fm
		Md	No

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# Pseudopotentials for Quantum-ESPRESSO

Pseudopotential's name  
gives information about :

- type of exchange-correlation functional
- type of pseudopotential
- e.g.:

`O.pbe-rrkjus.UPF`

Pseudopotential type: ULTRASOFT  
Method: Rappe Rabe Kaxiras Joannopoulos  
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr  
scalar relativistic

Origin: Original QE PP library  
Author: Andrea Dal Corso  
Generated by Andrea Dal Corso code (rrkj3)  
Uploaded by Layla Martin-Samos  
Classification controlled by Paolo Giannozzi

`O.pbe-van_ak.UPF`

Pseudopotential type: ULTRASOFT  
Method: Vanderbilt ultrasoft  
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr  
scalar relativistic

Origin: Original QE PP library  
Generated by Vanderbilt code version 7.3.4  
More Information: `O.pbe-van_ak.txt`  
Uploaded by Layla Martin-Samos  
Classification controlled by Paolo Giannozzi

`O.pbe-rrkjus.UPF` (details)

Perdew-Burke-Ernzerhof (PBE) exch-corr  
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)



Element &  $V_m$  for Quantum-ESPRESSO  
e.g, for calculation on  $\text{BaTiO}_3$ .

#### ATOMIC\_SPECIES

Ba 137.327 Ba.pbe-nsp-van.UPF

Ti 47.867 Ti.pbe-sp-van\_ak.UPF

O 15.999 O.pbe-van\_ak.UPF

- **ecutwfc**, **ecutrho** depend on type of pseudopotentials used (should test).
- When using ultrasoft pseudopotentials, set **ecutrho** =  $8-12 \times \text{ecutwfc}$  !!

- Element &  $V_{ion}$  for Quantum-ESPRESSO  
Should have **same exchange-correlation functional** for all pseudopotentials.

input

```
diagonalization = cg, mixing_mode  
mixing_beta = 0.7, conv_thr = 1.0  
/  
ATOMIC_SPECIES  
Fe 55.85 Fe pz-nd-rrkjus.UPF  
Co 58.93 Co pbe-nd-rrkjus.UPF  
ATOMIC_POSITIONS (crystal)  
Fe 0.00 0.00 0.00
```

oops!

output

```
Max angular momentum in pseudopotentials  
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%  
from readpp : error #          2  
inconsistent DFT read  
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%  
  
stopping ..█
```

# Pseudopotentials

## Quantum Espresso

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Not secure | www.pseudo-dojo.org

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# PSEUDŌ DŌJŌ

Download

3.13  
Mean

hints tests  
32.74 0.95  
37.25 2.20  
43.36 -0.09

Type

XC

Accuracy

Format

NC SR (ONCVSP v0.4)

PBE

standard

psp8

1 H 1  
32 0.1  
38 2.5  
42 -0.00  
Hydrogen

3 Li 2  
33 0.2  
37 1.9  
41 -0.10  
Lithium

11 Na 3  
38 0.4  
44 4.6  
48 -0.00  
Sodium

19 K 3  
33 0.2  
37 2.0  
43 -0.30  
Potassium

37 Rb 3  
19 0.2  
23 2.9  
29 -0.40  
Rubidium

55 Cs 3  
19 0.1  
25 1.5  
29 -0.40  
Caesium

87 Fr 3  
19 0.1  
25 1.5  
29 -0.40  
Francium

4 Be 2  
36 4.4  
44 4.4  
50 0.20  
Beryllium

12 Mg 3  
36 0.4  
42 1.5  
48 0.00  
Magnesium

20 Ca 3  
28 0.1  
34 0.3  
38 -0.20  
Calcium

38 Sr 3  
28 1.3  
34 6.1  
40 -0.20  
Strontium

56 Ba 3  
18 0.9  
22 4.9  
28 -0.10  
Barium

88 Ra 3  
18 0.9  
22 4.9  
28 -0.10  
Radium

21 Sc 4  
35 1.3  
39 2.3  
45 -0.00  
Scandium

39 Y 4  
30 1.0  
36 2.3  
42 -0.00  
Yttrium

71 Lu 4  
25 0.8  
29 0.8  
35 -0.00  
Lutetium

103 Lr 4  
25 0.8  
29 0.8  
35 -0.00  
Lawrencium

22 Ti 4  
38 0.9  
42 1.3  
46 -0.00  
Titanium

40 Zr 4  
29 0.9  
33 1.1  
39 -0.00  
Zirconium

72 Hf 4  
25 0.8  
29 0.8  
35 -0.00  
Hafnium

104 Rf 4  
25 0.8  
29 0.8  
35 -0.00  
Rutherfordium

23 V 4  
42 1.3  
46 1.6  
50 -0.10  
Vanadium

41 Nb 4  
37 1.3  
41 1.3  
45 -0.00  
Niobium

73 Ta 4  
25 0.7  
29 0.6  
35 -0.10  
Tantalum

105 Db 4  
25 0.7  
29 0.6  
35 -0.10  
Dubnium

24 Cr 4  
43 10.5  
47 18.1  
51 -0.00  
Chromium

42 Mo 4  
36 1.4  
40 1.0  
46 -0.10  
Molybdenum

74 W 4  
31 0.2  
37 0.1  
43 -0.00  
Tungsten

106 Sg 4  
31 0.2  
37 0.1  
43 -0.00  
Seaborgium

25 Mn 4  
45 8.0  
49 16.9  
53 -0.10  
Manganese

43 Tc 4  
38 1.6  
42 1.1  
48 -0.00  
Technetium

75 Re 4  
31 0.7  
37 0.4  
43 -0.10  
Rhenium

107 Bh 4  
31 0.7  
37 0.4  
43 -0.10  
Bohrium

26 Fe 4  
41 5.6  
45 9.2  
49 -0.10  
Iron

44 Ru 4  
40 2.1  
44 1.5  
50 -0.00  
Ruthenium

76 Os 4  
33 1.7  
37 0.9  
43 -0.10  
Osmium

108 Hs 4  
33 1.7  
37 0.9  
43 -0.10  
Hassium

27 Co 4  
42 1.0  
46 1.4  
50 -0.00  
Cobalt

45 Rh 4  
40 2.6  
44 2.1  
50 -0.00  
Rhodium

77 Ir 4  
30 1.5  
34 0.9  
40 -0.20  
Iridium

109 Mt 4  
30 1.5  
34 0.9  
40 -0.20  
Meitnerium

28 Ni 4  
45 1.1  
49 1.5  
53 -0.10  
Nickel

46 Pd 4  
41 1.1  
45 1.3  
49 -0.10  
Palladium

78 Pt 4  
38 0.6  
42 0.5  
46 -0.20  
Platinum

110 Ds 4  
38 0.6  
42 0.5  
46 -0.20  
Darmstadtium

29 Cu 4  
42 0.5  
46 0.9  
50 -0.10  
Copper

47 Ag 4  
37 0.3  
41 0.6  
45 -0.10  
Silver

79 Au 4  
32 1.3  
36 1.6  
40 -0.30  
Gold

111 Rg 4  
32 1.3  
36 1.6  
40 -0.30  
Roentgenium

30 Zn 4  
38 0.3  
42 0.8  
46 -0.10  
Zinc

48 Cd 4  
51 1.1  
55 3.6  
59 -0.00  
Cadmium

80 Hg 4  
27 0.7  
31 7.2  
35 -0.10  
Mercury

112 Cn 4  
27 0.7  
31 7.2  
35 -0.10  
Copernicium

31 Ga 3  
36 0.5  
40 1.5  
44 -0.00  
Gallium

49 In 3  
31 0.1  
35 0.2  
39 -0.10  
Indium

81 Tl 3  
27 0.1  
31 0.2  
35 -0.10  
Thallium

113 Nh 3  
27 0.1  
31 0.2  
35 -0.10  
Nihonium

32 Ge 3  
38 0.5  
42 1.0  
46 -0.00  
Germanium

50 Sn 3  
32 0.8  
36 0.8  
40 0.00  
Tin

82 Pb 3  
24 0.1  
28 0.1  
32 0.4  
36 -0.00  
Lead

114 Fl 3  
24 0.1  
28 0.1  
32 0.4  
36 -0.00  
Flerovium

33 As 3  
39 0.4  
43 0.7  
47 -0.00  
Arsenic

51 Sb 3  
36 0.8  
40 1.0  
44 0.00  
Antimony

83 Bi 3  
29 0.2  
33 0.4  
37 -0.00  
Bismuth

115 Mc 3  
29 0.2  
33 0.4  
37 -0.00  
Moscovium

34 Se 3  
43 0.5  
47 0.2  
51 -0.00  
Selenium

52 Te 3  
34 0.8  
38 0.8  
42 0.10  
Tellurium

84 Po 3  
28 0.3  
32 0.5  
36 -0.00  
Polonium

116 Lv 3  
28 0.3  
32 0.5  
36 -0.00  
Livermorium

35 Br 2  
19 0.6  
23 0.2  
27 -0.20  
Bromine

53 I 2  
31 0.4  
35 1.1  
39 0.00  
Iodine

85 At 3  
na na na  
na na na  
Astatine

117 Ts 3  
na na na  
na na na  
Tennessine

36 Kr 2  
22 0.0  
26 2.3  
30 -0.00  
Krypton

54 Xe 2  
22 0.0  
26 2.3  
30 -0.00  
Xenon

86 Rn 3  
32 2.4  
36 2.4  
40 -0.00  
Radon

F.A.Q. Contribute Papers About

Select the flavor and [format](#), then click "Download" to get the complete table of pseudos or choose a specific element. "HTML" gives full test results.

5 B 2  
34 0.3  
38 0.6  
44 0.00  
Boron

6 C 2  
37 0.1  
41 0.1  
45 0.10  
Carbon

7 N 2  
36 0.2  
42 0.4  
48 -0.10  
Nitrogen

8 O 2  
36 0.2  
42 0.4  
48 -0.20  
Oxygen

9 F 2  
36 0.1  
42 0.5  
48 -0.60  
Fluorine

13 Al 2  
16 0.5  
20 1.3  
26 -0.10  
Aluminium

14 Si 2  
14 0.1  
18 0.2  
24 -0.10  
Silicon

15 P 2  
18 0.1  
22 0.3  
26 -0.50  
Phosphorus

16 S 2  
20 0.0  
26 0.1  
32 -0.00  
Sulphur

17 Cl 2  
25 0.8  
29 3.1  
33 -0.30  
Chlorine

18 Ar 2  
29 0.0  
33 1.2  
37 -0.00  
Argon

39 He 2  
39 0.0  
45 4.2  
49 na  
Helium

10 Ne 2  
30 0.0  
34 1.7  
40 na  
Neon

19 Ar 2  
19 0.8  
23 0.2  
27 -0.20  
Argon

20 Kr 2  
22 0.0  
26 2.3  
30 -0.00  
Krypton

21 Xe 2  
22 0.0  
26 2.3  
30 -0.00  
Xenon

22 Rn 2  
32 2.4  
36 2.4  
40 -0.00  
Radon

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# Pseudopotentials

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### SG15 ONCV Potentials

The SG15 Optimized Norm-Conserving Vanderbilt (ONCV) pseudopotentials were generated using the code ONCVSP (Optimized Norm-Conserving Vanderbilt Pseudopotential) scalar-relativistic version 2.1.1, 03/26/2014 by D. R. Hamann. The code is available at [www.mat-simresearch.com](http://www.mat-simresearch.com) and the procedure is described in

D. R. Hamann, Phys. Rev. B 88, 085117 (2013)  
<http://link.aps.org/doi/10.1103/PhysRevB.88.085117>

The parameters of the SG15 potentials were optimized to reproduce the results of all-electron calculations with high accuracy, using the procedure described in

M. Schlipf and F. Gygi, Computer Physics Communications **196**, 36 (2015).  
<http://dx.doi.org/10.1016/j.cpc.2015.05.011>.


A set of fully relativistic potentials was generated by Peter Scherpelz. These potentials are available in UPF format. The relativistic pseudopotential file names include the letters "FR". The corresponding publication is

P. Scherpelz, M. Govoni, I. Hamada, G. Galli; J. Chem. Theory Comput. (2016)  
<http://dx.doi.org/10.1021/acs.jctc.6b00114>.

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