

Generation of a gipaw pseudopotential using Quantum ESPRESSO

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The aim of this short tutorial is to give you the tools for building your own pseudopotentials for gipaw calculations. The building of a reliable pseudopotential (psp) can be a difficult task (and time-consuming) so the idea is NOT to start a psp from scratch but to use parameters you could find in the literature (mainly using Quantum ESPRESSO library). An excellent tutorial written by Paolo Giannozzi can be found in the documentation of the atomic code (in `qe.6.x/atomic/Doc` you can find the [tutorial *pseudo_gen.pdf*](http://people.sissa.it/~dalcorsor/lectures/lecture_pseudo_sb_2009.pdf) and also <http://people.sissa.it/~dalcorsor/pslibrary/index.html>). We also recommend the article describing the pslibrary genesis (<http://people.sissa.it/~dalcorsor/pslibrary/index.html>).

So, we assume you have a (good) set of parameters for the *pseudization* but not the gipaw data set. For this exercise, you will need the `ld1.x` program.¹ In this short tutorial, we shall work on the oxygen with a *norm-conserving* psp (the easiest case, the database from Davide Ceresoli is an excellent starting point <https://sites.google.com/site/dceresoli/pseudopotentials>).

For PAW, we recommend to use the pslibrary (input files are provided). Then you will simply need to add two instructions for generating a gipaw data set:

```
&inputp
  lpaw=.true.,
  lgipaw_reconstruction=.true.,           Required for gipaw psp
  use_paw_as_gipaw=.true.,             paw projectors can be used as gipaw (instead of
  pseudotype=3,                          generating new ones)
  file_pseudopw='O.pbe-n-kjpaw_psl.1.0.0.UPF',
  author='ADC',
  lloc=-1,
  rcloc=1.1
  which_augfun='PSQ',
  rmatch_augfun_nc=.true.,
  nlcc=.true.,
  new_core_ps=.true.,
  rcore=0.7,
  tm=.true.
/
```

Then simply run the program:

```
ld1.x -in O.in
```

and you will obtain the UPF file (a standardized format for psp files) *O.pbe-n-kjpaw_psl.1.0.0.UPF*. We will come back on the parameters later in this tutorial.

0. Extracting parameters

The new UPF format includes now the whole input file used for the generation of psp. In this case, a simple copy/paste and you have a working input ready to go. You can then directly proceed to step 4. Unfortunately, old psp (D. Ceresoli psp) do include only partial information about the psp. What is proposed here is to proceed through each of the pseudo generation steps separately in order to explain all parameters and the pseudization process.

¹ This is the *atomic* project in the quantum espresso. To compile it use *make ld1* during the installation.

<div><PP_INFO> Generated using "atomic" code by A. Dal Corso (espresso distribution) Author: anonymous Generation date: 11Jul2007 O 0 The Pseudo was generated with a Non-Relativistic Calculation 1 1.4500000E+00 L component and cutoff radius for Local Potential nl pn l occ Rcut Rcut US E pseu 2S 1 0 2.00 1.450000000000 1.450000000000 -2.91141592981 2P 2 1 3.00 1.450000000000 1.450000000000 -1.79757641992 </PP_INFO> <PP_HEADER> 0 Version Number O Element NC Norm - Conserving pseudopotential F Nonlinear Core Correction SLA PW PBX PBC PBE Exchange-Correlation functional 6.000000000000 Z valence -30.28545848631 Total energy 0.000 0.000 Suggested cutoff for wfc and rho 1 Max angular momentum component 1095 Number of points in mesh 2 1 Number of Wavefunctions, Number of Projectors Wavefunctions nl l occ 2S 0 2.00 2P 1 3.00 </PP_HEADER> <PP_MESH> <PP_R> <PP_GIPAW_RECONSTRUCTION_DATA> <PP_GIPAW_FORMAT_VERSION> 0.1 </PP_GIPAW_FORMAT_VERSION> <PP_GIPAW_CORE_ORBITALS> 1 <PP_GIPAW_CORE_ORBITAL> [...] </PP_GIPAW_PS_ORBITAL> </PP_GIPAW_ORBITALS> </PP_GIPAW_RECONSTRUCTION_DATA></div>	<div>Date of generation</div> <div>Important parameters valence state $2s^2p^3$ and value of rcut for each orbital.</div> <div>Some input parameters</div> <div>This a PBE psp Valence Z=6 undocumented for ncpp</div> <div>Numerical data starts here</div> <div>PSP (PP) starts here</div> <div>GIPAW data starts here</div> <div>End of file</div>
--	--

1. All-electron calculation

The first step in any psp generation is the all-electron calculation (AE). ([01_ae](#)).

&input		
title	= 'O'	Not used
zed	= 8	Atomic number (Z)
rel	= 0	rel=0 non-relativistic, rel=1 semirelativistic
config	= '[He] 2s2 2p3 3d-1'	neutral atom is $2s^2 2p^4$, 3d-1 : unused orbital (see next step)
iswitch	= 1	iswitch =1 for AE, 2 for test, 3 for psp generation
dft	= 'PBE'	functional
/		

The valence configuration is chosen according to your knowledge of the valence state. A

generic valence state must be chosen in order to have a transferable psp but you can also build a very specific pseudo for a certain class of compounds. In the case of PAW (pslibrary), the neutral valence state is used $2s^2 2p^4$. At a later step, it will be check that the psp is able to reproduce other valence configurations. Here an ionic configuration had been used by the original author, but this is not necessary.

Run the program with

```
ld1.x -i O_AE.in
```

The output looks like

Program LD1 v.6.1 (svn rev. 13369) starts on 15Nov2017 at 0: 3:20

HEADER

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite

"P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);

URL <http://www.quantum-espresso.org>",

in publications or presentations arising from this work. More details at
<http://www.quantum-espresso.org/quote>

Parallel version (MPI), running on 1 processors

Reading input from O_AE.in

----- All-electron run -----

AE starts here

O

atomic number is 8.00

dft =PBE lsd =0 sic =0 latt =0 beta=0.20 tr2=1.0E-14

Exchange-correlation = PBE (1 4 3 4 0 0)

mesh =1711 r(mesh) = 99.53989 a.u. xmin = -7.00 dx = 0.00800

1 Ry = 13.60569193 eV

Z=8, ok for O

Values of some parameters

n l	nl	e(Ry)	e(Ha)	e(eV)
1 0	1S 1(2.00)	-39.1842	-19.5921	-533.1285
2 0	2S 1(2.00)	-2.9114	-1.4557	-39.6118
2 1	2P 1(3.00)	-1.7976	-0.8988	-24.4572

Orbitals found

final scf error: 6.7E-15 reached in 25 iterations

Etot = -148.682384 Ry, -74.341192 Ha, -2022.926716 eV

Total energy

Ekin = 148.315400 Ry, 74.157700 Ha, 2017.933638 eV

Encl = -344.872935 Ry, -172.436468 Ha, -4692.234912 eV

Eh = 63.524051 Ry, 31.762025 Ha, 864.288664 eV

Exc = -15.648899 Ry, -7.824450 Ha, -212.914106 eV

normalization and overlap integrals

**Good to have some idea of the
orbital « size ».**

s(1S/1S) = 1.000000 <r> = 0.1997 <r2> = 0.0539 r(max) = 0.1291

s(1S/2S) = -0.000000

s(2S/2S) = 1.000000 <r> = 1.0855 <r2> = 1.4155 r(max) = 0.8526

s(2P/2P) = 1.000000 <r> = 1.1100 <r2> = 1.5740 r(max) = 0.7808

----- End of All-electron run -----

You can play with the valence state to observe variation in the orbital energy eigenvalues. You can also force the search of empty orbitals (3d-1: disable the search of this orbital). For example, you can also try:

```
config      = '[He] 2s2 2p3 3d0'
```

And in the output, you can observe that a bound 3d state is found (reminder: a cationic configuration).

```
[...]
n l   nl      e(Ry)    e(Ha)    e(eV)
  0 0   1S 1( 2.00)  -39.1842  -19.5921  -533.1285
  0 0   2S 1( 2.00)   -2.9114   -1.4557  -39.6118
  1 1   2P 1( 3.00)  -1.7976   -0.8988  -24.4572
  2 2   3D 1( 0.00)  -0.1326   -0.0663   -1.8041
[...]
```

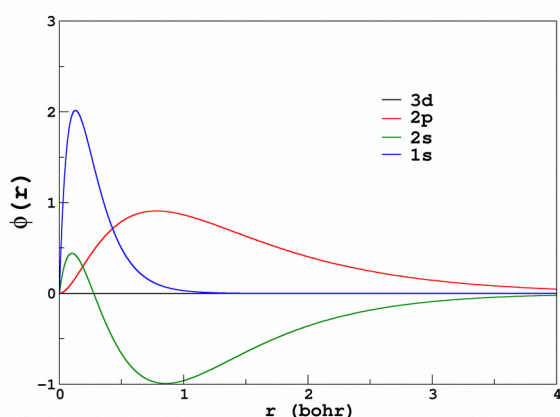


Figure 1: AE wave functions of O ($2s^2 2p^3$)

You can try different functionals to see how they affect the energy levels.

Here is a plot all AE orbitals (ld1.wfc); use xmgrace to plot them, type=NXYY (look the file header to determine the functions).

2. Pseudization

Go to [02a_pp_nc](#). We now pseudize the atom using a standard procedure (read documentation for more details).

```
&input
title      = 'O'
zed        = 8
rel        = 0
config     = '[He] 2s2 2p3 3d-1'
iswitch    = 3
dft        = 'PBE'
/
&inputp
pseudotype = 1
file_pseudopw = 'O.pbe-nc.UPF'
author      = 'TM'
lloc        = 2
tm          = .true.
lgipaw_reconstruction = .false.
```

Z=8: O
Non-relativistic
Pseudization valence configuration
Generate the pseudo
Functional

psp parameters
Norm-conserving
Name of the psp file
for posterity...
local component of the potential (here: d)
algorithm : Troullier-Martins (soft psp)
Not needed yet...

<pre> / 3 2S 1 0 2.00 0.00 1.45 1.45 0.0 2P 2 1 3.00 0.00 1.45 1.45 0.0 3D 3 2 -1.00 -1.79758 1.45 1.45 0.0 </pre>	<p>Pseudization parameters for each orbital</p> <p><i>nl N l occ E rcut rcut 0.00</i></p> <p><i>N : psp must be numbered</i></p> <p><i>occ : see config; last line for the local component</i></p> <p><i>E = 0.0 (atomic eigenvalue) or you can specify a energy (-1.00 = empty)</i></p> <p><i>rcut : at $r < rcut$ (r_c), the AE wave is replaced by a smooth function</i></p>
--	--

The general form of a pseudopotential is (so-called separable form²)

$$V_{ps}(r) = V_{loc}(r) + \sum_l |Y_{lm}\rangle \Delta V_{ps,l}(r) \langle Y_{lm}|$$

The reason of having the *d*-orbital in our calculation is because the latter is used to generate the local potential $V_{loc}(r)$. Other choices might be possible ($l=0$ or $l=1$) and the final one is generally determined after extensive transferability tests (see later).

```
ld1.x -i O_PP.in > O_PP.out
```

As outputs, you should have :

<i>ls -d1 *</i>	
<i>ld1ps.wfc</i>	<i>Pseudo (ps) wave-functions</i>
<i>ld1.test</i>	<i>Test of the pseudo with the reference electronic config</i>
<i>ld1.wfc</i>	<i>AE wave functions</i>
<i>O.pbe-nc.UPF</i>	<i>psp file</i>
<i>O_PP.in</i>	<i>input file</i>
<i>O_PP.out</i>	<i>output file</i>

O_PP.out :

<pre> Program LD1 v.6.1 (svn rev. 13369) starts on 15Nov2017 at 0:42:18 [...] Parallel version (MPI), running on 1 processors Reading input from O_PP.in ----- All-electron run ----- </pre>	<p>HEADER</p>
<pre> O atomic number is 8.00 dft =PBE lsd =0 sic =0 latt =0 beta=0.20 tr2=1.0E-14 Exchange-correlation = PBE (1 4 3 4 0 0) mesh =1095 r(mesh) = 99.04343 a.u. xmin = -7.00 dx = 0.01250 1 Ry = 13.60569193 eV n l nl e(Ry) e(Ha) e(eV) 1 0 1S 1(2.00) -39.1843 -19.5921 -533.1289 2 0 2S 1(2.00) -2.9114 -1.4557 -39.6118 2 1 2P 1(3.00) -1.7976 -0.8988 -24.4573 final scf error: 3.6E-15 reached in 25 iterations </pre>	<p>AE calculation</p>

² This form allows some simplifications in the calculation and a gain in computing time.

```

Etot =  -148.682753 Ry,  -74.341376 Ha,  -2022.931731 eV

Ekin =   148.315316 Ry,   74.157658 Ha,  2017.932501 eV
Encl =  -344.872753 Ry, -172.436376 Ha, -4692.232430 eV
Eh  =   63.523934 Ry,  31.761967 Ha,  864.287070 eV
Exc  =  -15.649250 Ry,  -7.824625 Ha, -212.918872 eV

```

normalization and overlap integrals

```

s(1S/1S) = 1.000000 <r> = 0.1997 <r2> = 0.0539 r(max) = 0.1298
s(1S/2S) = -0.000000
s(2S/2S) = 1.000000 <r> = 1.0855 <r2> = 1.4155 r(max) = 0.8569
s(2P/2P) = 1.000000 <r> = 1.1100 <r2> = 1.5740 r(max) = 0.7851

```

----- End of All-electron run -----

----- Generating NC pseudopotential -----

PSP generation

Generating local pot.: lloc=2, matching radius rcloc = 1.4500

V_{loc} first

Wfc 2S rcut= 1.449 Using Troullier-Martins method

2s orbital pseudization

Wfc 2P rcut= 1.449 Using Troullier-Martins method

2p orbital pseudization

```

The bmat matrix
1.35036  0.00000
0.00000 -1.16037

```

See the Theory...

----- End of pseudopotential generation -----

----- All-electron run -----

AE (again...)

[...]

----- End of All-electron run -----

----- Testing the pseudopotential -----

Testing the psp with the reference electronic configuration (**config**)

O

```

atomic number is 8.00 valence charge is 6.00
dft =PBE lsd=0 sic=0 latt=0 beta=0.20 tr2=1.0E-14
mesh =1095 r(mesh) = 99.04343 xmin = -7.00 dx = 0.01250

```

2 core (frozen) electrons
6 valence electrons

```

n l   nl      e AE (Ry)    e PS (Ry)  De AE-PS (Ry)
1 0   2S  1( 2.00)  -2.91142   -2.91142    0.00000
2 1   2P  1( 3.00)  -1.79758   -1.79758   -0.00000

```

Comparison between ϵ_{AE} and ϵ_{PS}
By construction, the $\Delta\epsilon$ should be 0.

eps = 6.7E-16 iter = 6

```

Etot =  -148.682753 Ry,  -74.341376 Ha,  -2022.931731 eV
Etotps = -30.285346 Ry,  -15.142673 Ha,  -412.053089 eV

```

```

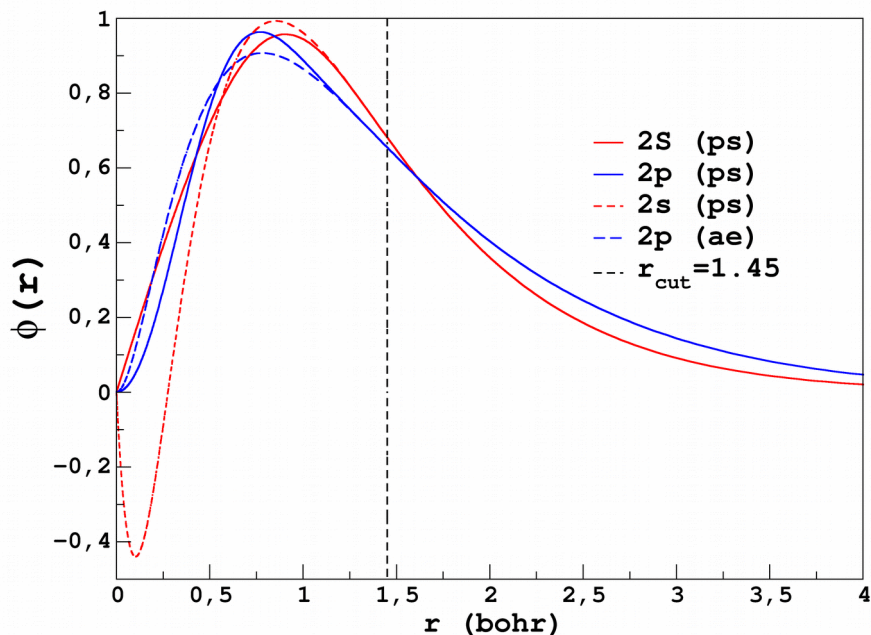
Ekin =   18.978597 Ry,   9.489299 Ha,  258.216950 eV
Encl =  -63.612035 Ry, -31.806017 Ha, -865.485751 eV
Ehrt =   20.708134 Ry,  10.354067 Ha,  281.748493 eV
Ecxc =   -5.579689 Ry,  -2.789845 Ha, -75.915535 eV
Epseu=   -0.780353 Ry,  -0.390177 Ha, -10.617246 eV

```

----- End of pseudopotential test -----

END

Below is a figure with the AE/PS wave functions :



Pseudo and AE wavefunction of the oxygen ($2s^2 2p^3$ $r_c=1.45$ bohr, Troullier-Martins)

As you can observe, below the cutoff radius r_c the AE wfct is replaced by a smooth function (thus less expensive in terms of plane-wave function expansion). At r_c , wave functions match up to the fourth order derivative.

3. Testing the pseudopotential

02b_pp_nc_test

The input file is O_PP.in; we test the transferability of our psp using 4 valence configurations:

```
&input
title      = 'O'
zed        = 8
rel        = 0
config     = '[He] 2s2 2p3 3d-1'
iswitch    = 2
dft        = 'PBE'
/
&inputp
pseudotype = 1
file_pseudopw = 'O.pbe-nc.UPF'
author     = 'TM'
lloc       = 2
tm         = .true.
```

2 :TEST

PSP definition

```

lgipaw_reconstruction = .false.
/
3
2S 1 0 2.00 0.00 1.45 1.45 0.0
2P 2 1 3.00 0.00 1.45 1.45 0.0
3D 3 2 -1.00 -1.79758 1.45 1.45 0.0

&test
nconf      = 4
file_pseudo = 'O.pbe-nc.UPF'
/
2
2S 1 0 1.90 -0.60 1.45 1.45 0.0
2P 2 1 2.70 -0.60 1.45 1.45 0.0
2
2S 1 0 2.00 -0.40 1.45 1.45 0.0
2P 2 1 3.00 -0.40 1.45 1.45 0.0
2
2S 1 0 2.00 -0.20 1.45 1.45 0.0
2P 2 1 3.20 -0.20 1.45 1.45 0.0
2
2S 1 0 2.00 -0.10 1.45 1.45 0.0
2P 2 1 3.50 -0.10 1.45 1.45 0.0

```

not yet...

PS electronic configuration

Local component

Test start here
4 testing configurations
psp file used

config#1 : 2 orbitals

2s^{1.90}

2p^{2.70}

config#2 : 2 orbitals

2s^{2.00}

2p^{3.00}

config#3 : 2 orbitals

2s^{2.00}

2p^{3.20}

config#4 : 2 orbitals

2s^{12.00}

2p^{3.50}

The output file contains:

```

Program LD1 v.6.1 (svn rev. 13369) starts on 15Nov2017 at 1: 8:43
[...]
Reading input from O_PP.in
----- All-electron run -----
[...]
----- End of All-electron run -----

----- Testing the pseudopotential -----

O

atomic number is 8.00 valence charge is 6.00
dft =PBE lsd =0 sic =0 latt =0 beta=0.20 tr2=1.0E-14
mesh =1095 r(mesh) = 99.04343 xmin = -7.00 dx = 0.01250

n l nl e AE (Ry) e PS (Ry) De AE-PS (Ry)
1 0 2S 1( 1.90) -3.43655 -3.43852 0.00197
2 1 2P 1( 2.70) -2.32199 -2.31910 -0.00289

eps = 1.1E-15 iter = 13

Etot = -147.748557 Ry, -73.874279 Ha, -2010.221355 eV
Etotps = -29.351439 Ry, -14.675720 Ha, -399.346640 eV

Ekin = 18.177417 Ry, 9.088708 Ha, 247.316332 eV
Encl = -59.774344 Ry, -29.887172 Ha, -813.271306 eV
Ehrt = 18.067761 Ry, 9.033880 Ha, 245.824387 eV
Ecxc = -5.157721 Ry, -2.578860 Ha, -70.174359 eV
Epseu = -0.664552 Ry, -0.332276 Ha, -9.041694 eV

----- End of pseudopotential test -----

```

BLA BLA BLA ...

AE

TEST with
the first testing configuration

few ~mRy : Ok !

----- All-electron run -----

AE

[...]

----- End of All-electron run -----

----- Testing the pseudopotential -----

Second configurations

O

atomic number is 8.00 valence charge is 6.00
dft =PBE lsd =0 sic =0 latt =0 beta=0.20 tr2=1.0E-14
mesh =1095 r(mesh) = 99.04343 xmin = -7.00 dx = 0.01250

n	l	nl	e AE (Ry)	e PS (Ry)	De AE-PS (Ry)
1	0	2S 1(2.00)	-2.91142	-2.91142	0.00000
2	1	2P 1(3.00)	-1.79758	-1.79758	-0.00000

[...]

----- End of pseudopotential test -----

----- All-electron run -----

AE

[...]

----- End of All-electron run -----

----- Testing the pseudopotential -----

Third configuration

O

atomic number is 8.00 valence charge is 6.00
dft =PBE lsd =0 sic =0 latt =0 beta=0.20 tr2=1.0E-14
mesh =1095 r(mesh) = 99.04343 xmin = -7.00 dx = 0.01250

n	l	nl	e AE (Ry)	e PS (Ry)	De AE-PS (Ry)
1	0	2S 1(2.00)	-2.66149	-2.66068	-0.00081
2	1	2P 1(3.20)	-1.54966	-1.55095	0.00129

< 1 mRy : perfect
Ok.

[..]

----- End of pseudopotential test -----

----- All-electron run -----

[...]

----- End of All-electron run -----

----- Testing the pseudopotential -----

Config #3

O

atomic number is 8.00 valence charge is 6.00
dft =PBE lsd =0 sic =0 latt =0 beta=0.20 tr2=1.0E-14
mesh =1095 r(mesh) = 99.04343 xmin = -7.00 dx = 0.01250

n	l	nl	e AE (Ry)	e PS (Ry)	De AE-PS (Ry)
1	0	2S 1(2.00)	-2.30368	-2.30149	-0.00219
2	1	2P 1(3.50)	-1.19694	-1.19922	0.00229

~ mRy : ok
~ mRy : ok

[...]

----- End of pseudopotential test -----

The test consists of comparing the energy eigenvalues of the orbitals between a AE calculation and calculation with the psp. Here all tests passed well; thus at least we are somewhat confident that our pseudo is good for configurations with small variations on 2s (you can perform more extensive tests) and 2p population varying from 2.7 to 3.5.

Generally, psp are benchmarked with reference compounds or compared to AE calculations.

4. The GIPAW potential

We can now proceed to the next step, and you will generate you first gipaw psp! In the input, we need to add a section that gives the parameters for construction the gipaw projectors: two projectors at least for each angular quantum number l .

<pre>&input title = 'O' zed = 8 rel = 0 config = '[He] 2s2 2p3 3d-1 3s-1 3p-1' iswitch = 3 dft = 'PBE' /</pre>	The additional orbitals will be used to construct the second gipaw-projector (see below)
<pre>&inputp pseudotype = 1 file_pseudopw = 'O.pbe-nc.UPF' author = 'TM' lloc = 2 tm = .true. lgipaw_reconstruction = .true. /</pre>	PSP definition
<pre>3 2S 1 0 2.00 0.00 1.45 1.45 0.0 2P 2 1 3.00 0.00 1.45 1.45 0.0 3D 3 2 -1.00 -1.79758 1.45 1.45 0.0 &test /</pre>	PSP parameters
<pre>4 2S 1 0 2.00 0.00 1.45 1.45 0.0 3S 1 0 0.00 0.00 1.45 1.45 0.0 2P 2 1 3.00 0.00 1.45 1.45 0.0 3P 2 1 0.00 0.00 1.45 1.45 0.0</pre>	&test = start of the gipaw section 4 projectors (2S:2+2P:2) 2S#1 2S#2 2P#1 2P#2

Run the program and then you can test you gipaw psp in an NMR calculation.

As an extra, you can try to repeat the whole procedure for Si.