

# HOWTO generate the same PAW atomic data with USPP and AtomPAW

Example on Iron

Keywords in **bold** do not have to be changed for a comparison with AtomPAW

## fe\_ae\_d7s1.adat USPP file

	<b>1</b> 0 0 0 3	ifae,ifpsp,ifprt,ifplw,ilogd
$\Gamma_{PAW}$	2.0 <b>-5.0 5.0 200</b>	rlogd,emin,emax,nnt
	1.0d-10 1.0d-09 0.2 0	thresh,tol,damp,maxit
$Z$	iron	title
$r_{max}$	26.0 0.00 5.0	z,xion,exfact
	200.0 5.11 165.45	rmax,aasf,bbsf
Total nb of states	8 2	ncspvs,irel
0 for nonrelativistic 2 for scalarrelativistic	100 2.000 -515.0	nnlz,wnl,ee
	200 2.000 -60.5	nnlz,wnl,ee
	210 6.000 -51.5	nnlz,wnl,ee
	300 2.000 -7.0	nnlz,wnl,ee
	310 6.000 -4.5	nnlz,wnl,ee
	320 7.000 -1.0	nnlz,wnl,ee
	400 1.000 -0.5	nnlz,wnl,ee
	410 0.000 -0.2	nnlz,wnl,ee

*These are hidden values in AtomPAW*

*0 for LDA-PW  
5 for GGA-PBE*

*Where  $r_0$  is printed in AtomPAW output file*

## fe\_ps.adat USPP file

	<b>0</b> 2 1 1 3	ifae,ifpsp,ifprt,ifplw,ilogd
$\Gamma_{PAW}$	2.0 <b>-5.0 5.0 200</b>	rlogd,emin,emax,nnt
	1.0d-10 1.0d-09 0.2 0	thresh,tol,damp,maxit
	iron	title
Nb of core states (nb of "c" in AtomPAW)	3 5 3	ncores,nvales,nang
Nb of valence states (nb of "v" in AtomPAW)	10.0 20.0 40.0 10.0	besrmax,besemin,besemax,besde
	3 1 2.0 1.95	keyps,ifpcor,rinner,rpcore
$r_{core}$	6 1.9	nbeta,rcloc
$rc_s, rc_p, rc_d, rc_f$	2.0 2.0 2.0	rc
First s partial wave (valence state #1)	0 1 0.0 2	l1l,keyee,eeread,iptype
2nd s partial wave (valence state #4)	0 4 0.0 2	l1l,keyee,eeread,iptype
First p partial wave (valence state #2)	1 2 0.0 2	l1l,keyee,eeread,iptype
2nd p partial wave (valence state #5)	1 5 0.0 2	l1l,keyee,eeread,iptype
First d partial wave (valence state #3)	2 3 0.0 2	l1l,keyee,eeread,iptype
2nd d partial wave (additional) at $E_{ref}=2.0$ Ry	2 0 2.0 2	l1l,keyee,eeread,iptype
	8 10.0	npf,ptryc
$l_{loc}$	3 0 0.0 1	lloc,keyee,eloc,iplotype
$E_{loc}$	3 8 10.0	ifqopt,nqf,qtryc

*Change only if necessary!*

Total number of partial waves =  
Nb of valence states  
+ Nb of additional partial waves

*1 for ultrasoft  
3 for trouilliermartins*

## Uspp2abinit.dat USPP

	SHAPETYPE= 2	1 for sinc 2 for besselsshape
	RCOMPFACT= 0.95	RCOMPFACT= $\Gamma_{shape}/\Gamma_{PAW}$
Mandatory for the comparison with AtomPAW	<b>OPT_TCORE=1</b>	
	ECUT_RSO= 10.	
	WERROR_RSO= 0.0005	Real Space Optimization: Same values as those asked by AtomPAW2Abinit (Comment for no real space optimization)
	GAMMAFACT_RSO= 2.	

# Fe.atompaw.input file

**Z** ←

```

Fe 26
GGA-PBE finite-nucleus scalarrelativistic loggrid 1500 200. 2.
4 4 3 0 0 0
3 2 7
4 0 1
4 1 0
0 0 0
c
c
v
v
c
v
v
v
2
2. 1.9 1.9 1.95
n
n
y
2.0
n
custom polynom2 7 10. vanderbiltortho besselshape
3.0. ultrasoft
2.0
2.0
2.0
2.0
2.0
2.0
1
3 2 6
4 0 2
0 0 0
0
  
```

See *exfac* USPP argument

$n_{\max}^s, n_{\max}^p, n_{\max}^d, n_{\max}^f$

See *irel* USPP argument

Electronic configuration corresponding to the one in \*\_ae.adat USPP file

Value to be chosen by user  
Then  $r_0$  value (printed in output) has to be used to define *aasf* and *bbsf* USPP arguments

$r_{\max}$   $r_{PAW}$

Core and valence states  
See *ncspvs* USPP argument

$r_{\max}$   $r_{PAW}$   $r_{shape}$   $r_{Vloc}$   $r_{core}$

No additional s partial wave

No additional p partial wave

Additional d partial wave at  $E_{ref}=2.0$  Ry

$r_{loc}$   $E_{loc}$   $r_{cs}$   $r_{cp}$   $r_{cd}$

See *iploctype* USPP argument:  
ultrasoft is *iploctype*=1  
trouillermartins is *iploctype*=3

$p = (ptryc-1)$   $q_{cut}$

sinc is SHAPETYPE=1  
besselshape is SHAPETYPE=2  
in *uspp2abinit.dat*

Test configuration, if wanted

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