

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

	1	0	0	0	3	ifae,ifpsp,ifprt,ifplw,ilogd
Γ_{PAW}	2.0	-5.0	5.0	200		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
Electronic configuration	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

Annotations for fe_ae_d7s1.adat USPP file:

- $1+l_{max}$ points to the 3 in the first row.
- $1/(r_0.Z)$ points to the 200 in the second row.
- $-\ln(r_0.Z)$ points to the 5.0 in the second row.
- 0 for LDA-PW, 5 for GGA-PBE points to the 2 in the sixth row.
- Where r_0 is printed in AtomPAW output file points to the 5.11 in the sixth row.

fe_ps.adat USPP file

	0	2	1	1	3	ifae,ifpsp,ifprt,ifplw,ilogd
Γ_{PAW}	2.0	-5.0	5.0	200		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
r_{core}	3	1	2.0	1.95		keyps,ifpcor,rinner,rpcore
rc_s, rc_p, rc_d, rc_f	6	1.9				nbeta,rcloc
First s partial wave (valence state #1)	2.0	2.0	2.0			rc
2nd s partial wave (valence state #4)	0	1	0.0	2		l1l,keyee,eeread,iptype
First p partial wave (valence state #2)	0	4	0.0	2		l1l,keyee,eeread,iptype
2nd p partial wave (valence state #5)	1	2	0.0	2		l1l,keyee,eeread,iptype
2nd d partial wave (valence state #3)	1	5	0.0	2		l1l,keyee,eeread,iptype
2nd d partial wave (additional) at $E_{ref}=2.0$ Ry	2	3	0.0	2		l1l,keyee,eeread,iptype
l_{loc}	2	0	2.0	2		l1l,keyee,eeread,iptype
E_{loc}	8	10.0				npf,ptryc
	3	0	0.0	1		lloc,keyee,eloc,iplotype
	3	8	10.0			ifqopt,nqf,qtryc

Annotations for fe_ps.adat USPP file:

- $1+l_{max}$ points to the 3 in the first row.
- $1+l_{max}$ points to the 200 in the second row.
- $1+l_{max}$ points to the 3 in the sixth row.
- $1+l_{max}$ points to the 1.95 in the seventh row.
- Γ_{Vloc} points to the 1.9 in the eighth row.
- Total number of partial waves = Nb of valence states + Nb of additional partial waves points to the 2 in the ninth row.
- $1+p$ points to the 2 in the tenth row.
- q_{cut} points to the 2 in the eleventh row.
- 1 for ultrasoft, 3 for trouilliermartins points to the 1 in the twelfth row.
- Change only if necessary! points to the 10.0 in the thirteenth row.

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	OPT_TCORE=1	
	USE_XC_NHAT=0	
This is asked by AtomPAW2Abinit (include compensation in XC or not ?)	ECUT_RSO= 10.	Real Space Optimization: Same values as those asked by AtomPAW2Abinit (Comment for no real space optimization)
	WERROR_RSO= 0.0005	
	GAMMAFACT_RSO= 2.	

Fe.atompaw.input file

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Z
See exfac
USPP argument
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

```

$n_{max}^s, n_{max}^p, n_{max}^d, n_{max}^f$
 r_{max}
 r_{PAW}
 r_{shape}
 r_{Vloc}
 r_{core}
 r_{loc}
 E_{loc}
 r_{cs}
 r_{cp}
 r_{cd}
 $p = (pt_{ryc}-1)$
 q_{cut}
 r_0 value (printed in output) has to be used to define *aasf* and *bbsf* USPP arguments
 Core and valence states
 See *ncspvs* USPP argument
 Additional d partial wave at $E_{ref}=2.0$ Ry
 See *iploctype* USPP argument:
 ultrasoft is *iploctype*=1
 trouillermartins is *iploctype*=3
 sinc is SHAPETYPE=1
 besselshape is SHAPETYPE=2
 in *uspp2abinit.dat*
 Test configuration, if wanted

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