

PDOS calculation tool : fmpdos

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In order to plot pdos for different orbitals of different species one tool `fmpdos` can be used. This tool is implemented in the siesta-3.2. This is a direct tool which can be compiled in the directory : `~/siesta-3.2/Util/Contrib/APostnikov` using command :

```
~/siesta-3.2/Util/Contrib/APostnikov$ make
```

You can copy generated binary file `fmpdos` in `~/bin` directory using :

```
~/siesta-3.2/Util/Contrib/APostnikov$ cp fmpdos ~/bin
```

Now go to the directory where *.PDOS file has been generated using conventional method. e.g. By adding related block :

```
%block Projected-density-of-states
```

```
-30.00 15.00 0.200 500 eV
```

```
%endblock Projected-density-of-states
```

in `fdf` file and siesta run. This will generate `systemlable.pdos` in the energy range -30.0 to 15.0 eV in the working directory.

Here I am using the example of `peo5-LiI-lda` system. Before `fmpdos` run one must know about PDOS file name. Here it is “`peorel5-liI-lda.PDOS`” and “Atom index” which is given in `fdf` file :

In my case :

```
%block ChemicalSpeciesLabel
```

```
1      6      C
```

```
2      1      H
```

```
3      8      O
```

```
4      3      Li
```

```
5     53      I
```

```
%endblock ChemicalSpeciesLabel
```

The s electronic configuration of species is also important, in order to know the valance orbitals . The

details are mentioned in table-1.

Table-1

Atom index	Name of Species with atomic number	Electronic configuration	Valence cell for PDOS cancellation
1	C-6	1s2, 2s2 2p2	2s2 2p2 n=2, l=0,1
2	H-1	1s1	1s1 n=1 l=0
3	O-8	1s2, 2s2 2p4	2s2 2p4 n=2, l=0, 1
4	Li-3	1s2, 2s1	2s1, 2p0 n=2 l=0, 1
5	I-53,5s1	5s1,5p0 n=5, l=0, 1

Now in the working dir , where the PDOS file is available use command :

[drmohanlv@localhost peo5-LiI-lda-opt]\$ fmpdos

An input file name will be asked.

```

[drmohanlv@localhost peo5-LiI-lda-opt]$ fmpdos
Input file name (PDOS):
peo5-LiI-lda.PDOS
Output file name :
C~C
[drmohanlv@localhost peo5-LiI-lda-opt]$ fmpdos
Input file name (PDOS):

```

After giving input file name subsequent output file name will also be asked. This file name may be of your choice. I have given pdosC2s.dat for 2s orbital of Carbon atom .

```

Applications Places System [Icons] [Network] [System] [Sun Jun 8, 5:58 PM] Dr Mohan L Verma
drmhnanlv@localhost: ~/peo5-LiI-lda-opt
File Edit View Search Terminal Help
C.ion.xml      NON TRIMMED_KP_LIST  peorel5-LiI-lda.DM
CLOCK          OCCS                 peorel5-LiI-lda.DOS
C.psf          0.ion              peorel5-LiI-lda.EIG
fdf.log        0.ion.xml          peorel5-LiI-lda.FA
field          0.psf              peorel5-LiI-lda.KP
FORCE_STRESS   pdosAg4d.dat       peorel5-LiI-lda.PDOS
fort.48        pdosC1s.dat        peorel5-LiI-lda.RHO
H.ion          pdos.dat           peorel5-LiI-lda.STRUCT_NEXT_ITER
H.ion.xml      pdosLi2s.dat       peorel5-LiI-lda.STRUCT_OUT
H.psf          pdos.xml           peorel5-LiI-lda.xml
I.ion          peo5-LiI-lda        peorel5-LiI-lda.XSF
I.ion.xml      peo5-LiIm.xyz       peorel5-LiI-lda.XV
INPUT_TMP.403589736 peorel5-agi.fdf    peorel5-LiI-lda.xyz
INPUT_TMP.403619976 peorel5-agi.fdf~   rho2xsf
INPUT_TMP.473340166 peorel5-agi.out    siesta
INPUT_TMP.496033915 peorel5-LiI-lda.alloc vibra
[drmhnanlv@localhost peo5-LiI-lda-opt]$ fmpdos
  Input file name (PDOS):
peorel5-LiI-lda.PDOS
  Output file name :
pdosC2s.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):

```

After that the details of orbitals/suborbitals will be asked as :

```

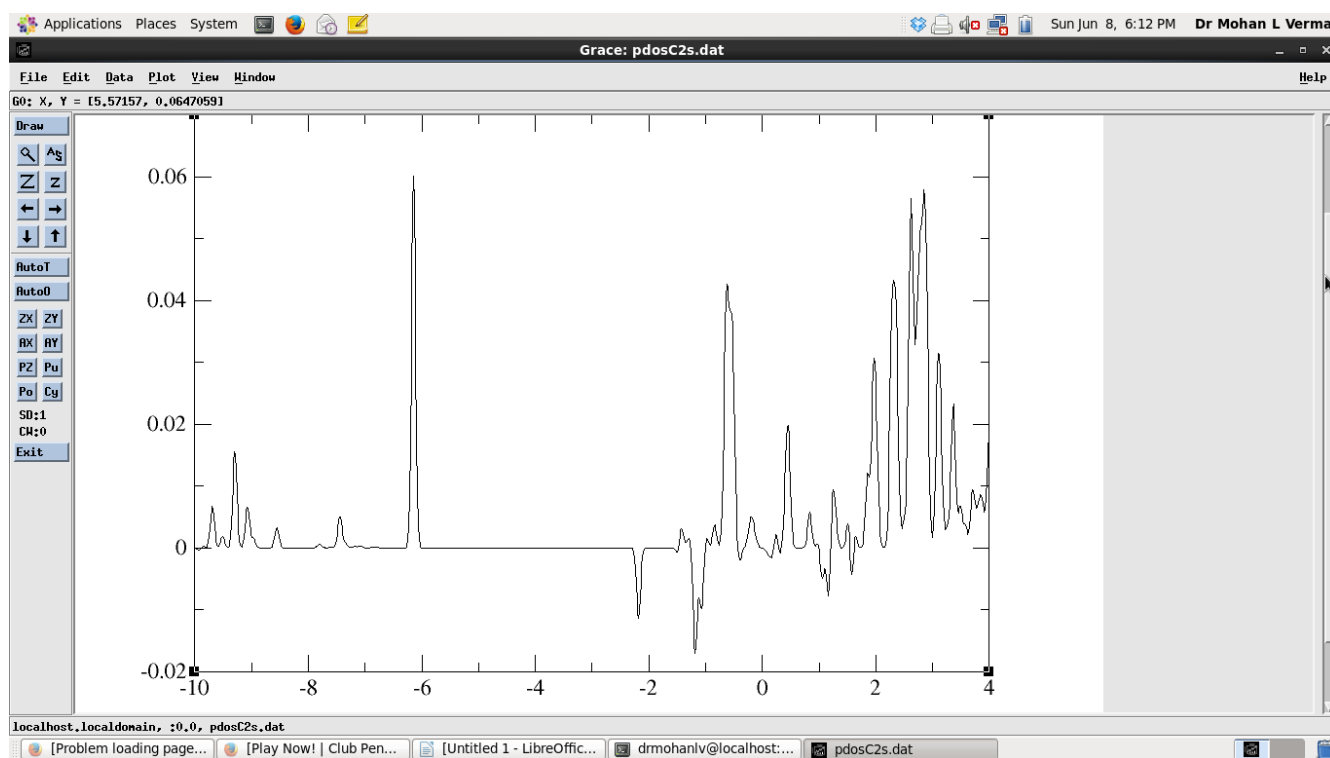
Applications Places System [Icons] [Network] [System] [Sun Jun 8, 5:47 PM] Dr Mohan L Verma
drmhnanlv@localhost: ~/peo5-LiI-lda-opt
File Edit View Search Terminal Help
C.ion          Li.psf             peorel5-LiI-lda.DM
C.ion.xml      NON TRIMMED_KP_LIST peorel5-LiI-lda.DOS
CLOCK          OCCS                 peorel5-LiI-lda.EIG
C.psf          0.ion              peorel5-LiI-lda.FA
fdf.log        0.ion.xml          peorel5-LiI-lda.KP
field          0.psf              peorel5-LiI-lda.PDOS
FORCE_STRESS   pdosAg4d.dat       peorel5-LiI-lda.RHO
fort.48        pdos.dat           peorel5-LiI-lda.STRUCT_NEXT_ITER
H.ion          pdosLi2s.dat       peorel5-LiI-lda.STRUCT_OUT
H.ion.xml      pdos.xml           peorel5-LiI-lda.xml
H.psf          peo5-LiI-lda        peorel5-LiI-lda.XSF
I.ion          peo5-LiIm.xyz       peorel5-LiI-lda.XV
I.ion.xml      peorel5-agi.fdf    peorel5-LiI-lda.xyz
INPUT_TMP.403589736 peorel5-agi.fdf~   rho2xsf
INPUT_TMP.403619976 peorel5-agi.out    siesta
INPUT_TMP.473340166 peorel5-LiI-lda.alloc vibra
INPUT_TMP.496033915 peorel5-LiI-lda.ANI
[drmhnanlv@localhost peo5-LiI-lda-opt]$ pwd
/home/drmhnanlv/peo5-LiI-lda-opt
[drmhnanlv@localhost peo5-LiI-lda-opt]$ fmpdos
  Input file name (PDOS):
peorel5-LiI-lda.PDOS
  Output file name :
pdosC1s.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
1
  Extract data for n= ... (0 for all n ):
2
  Extract data for l= ... (-1 for all l ):
0
  Extract data for m= ... (9 for all m ):
9
[drmhnanlv@localhost peo5-LiI-lda-opt]$

```

Here species index -1 for carbon is given. And pdos is calculated for n=2 and l=0 for S orbital.

Finally a data file “pdosC2s.dat” is obtained, which can be plotted using xmgrace using

[drmhnanlv@localhost peo5-LiI-lda-opt]\$ xmgrace pdosC2s.dat



Now rerun for C2p, O2s, O2p and other orbitals given in the table-1.

All the best.
