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 cammand :

~/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.

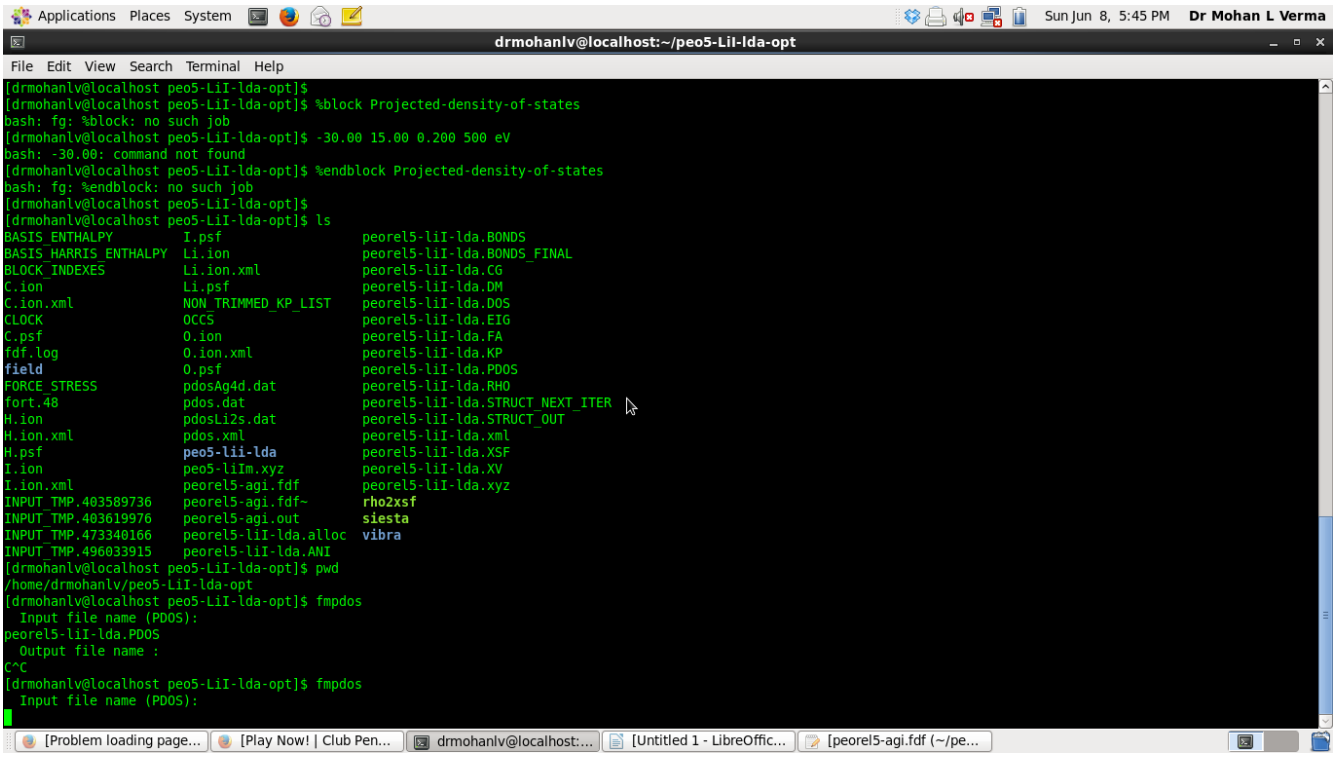
Table-1

Atom index	Name of Species with atomic number	Electronic configuration	Valence cell for PDOS canculation
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

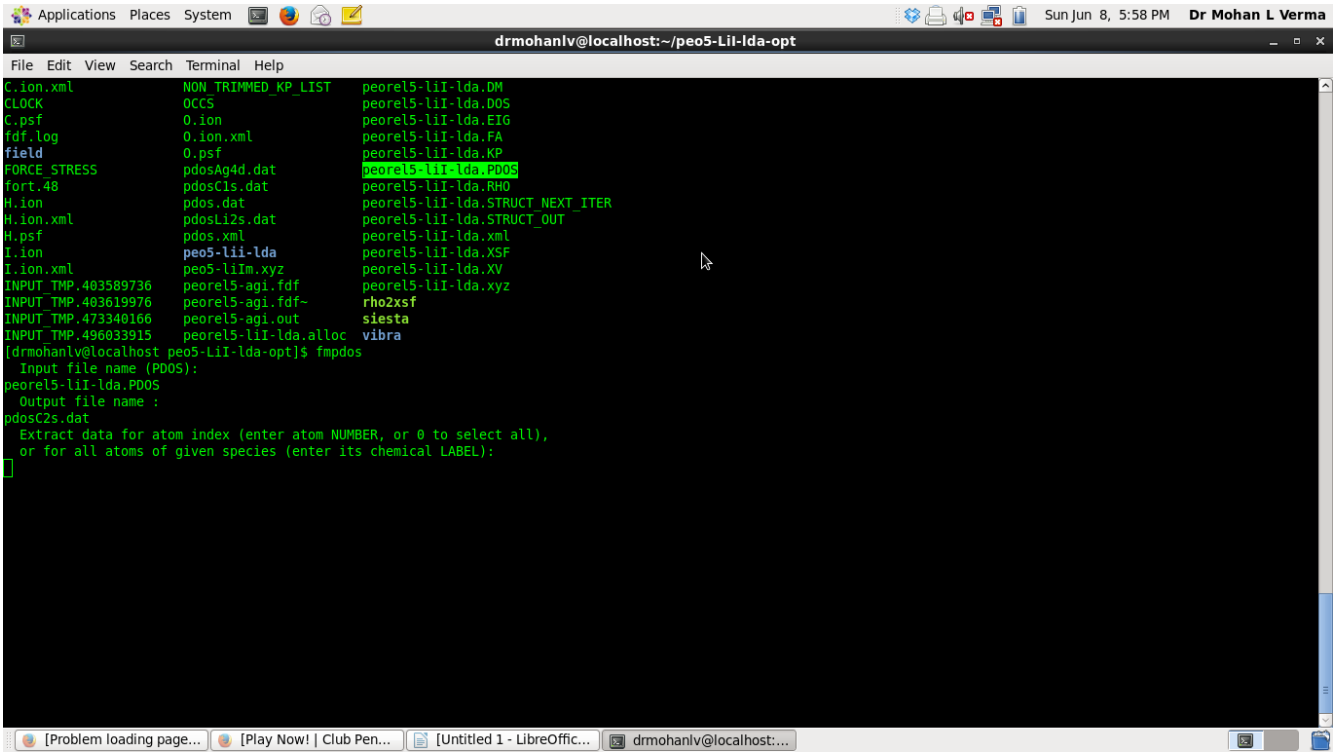
Now in the working dir , where the PDOS file is available use command :

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

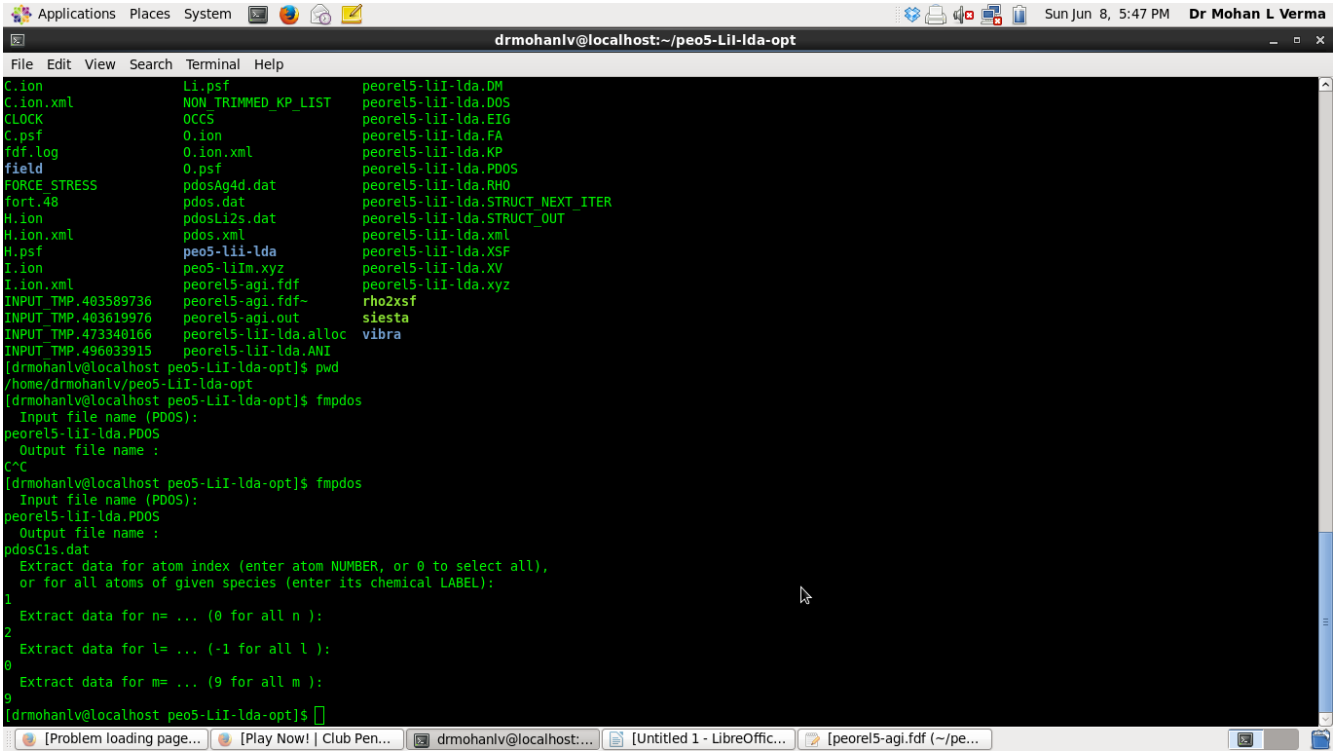
An input file name will be asked.



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 .



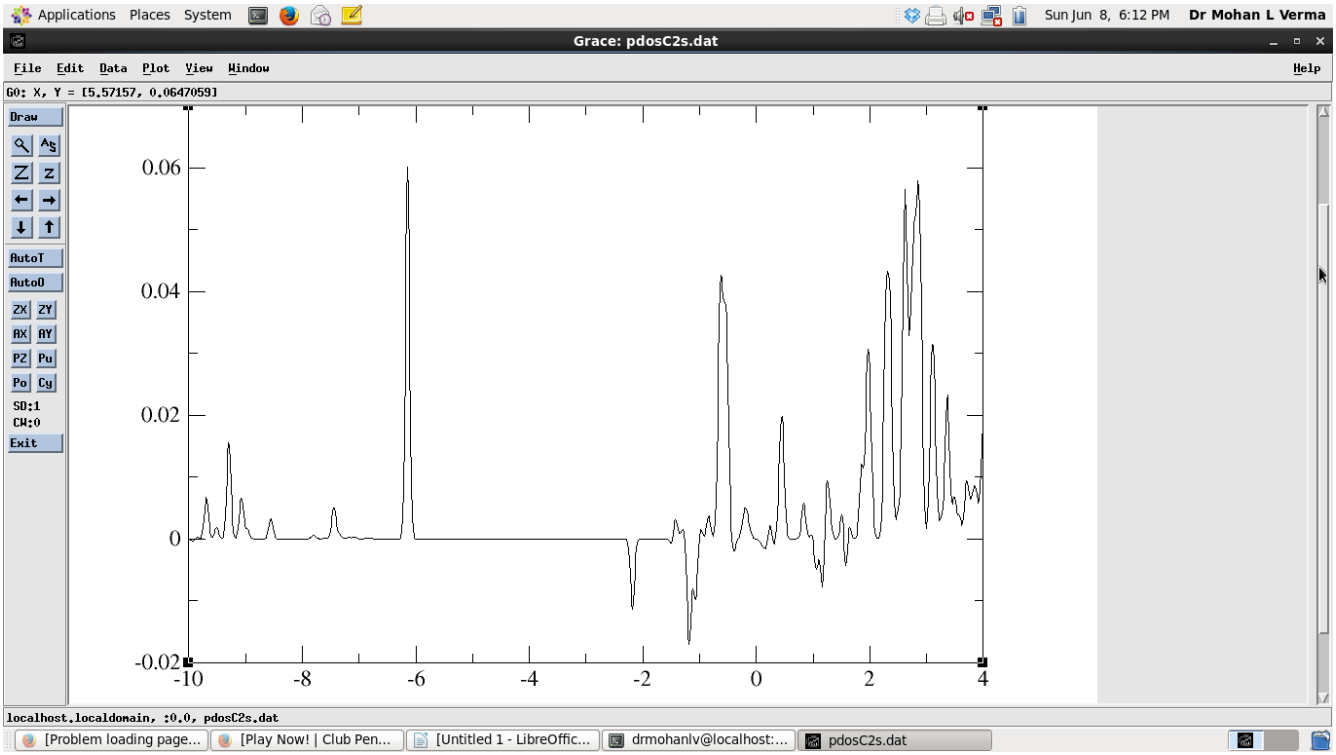
After that the details of orbitals/suborbitals will be asked as :



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

[drmohanlv@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.

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