COOP Utility how to use ?

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This utility is available in ~/siesta/Util/COOP.

If your siesta has been successfully compiled, then using simple "make" command in this directory, one can get required *mprop* binary file. Copy this binary file in your working directory for coop/cohp/pdos analysis of your system under study.

In order to start using coop utility first of all you have to add :

COOP.Write .true.

In your input *.fdf file.

After a successful siesta run, this will generate all required files i.e. *.HSX and *.WFSX in working directory. For further coop analysis, make a directory COOP and copy *.HSX, *.WFSX file and mprop compiled in ~siesta/Util/COOP in this directory.

Now let us create two different input files for coop/cohp as well as PDOS study.

Here I am giving you one example of BATIO3 taken from siesta-L.

(a) For COOP/COHP study

make a text file entitled as *coo.mpr* containing following :

BaTiO3 # Name of the siesta output files (as in SystemLabel)

COOP # calculation is a COOP analysis (could be DOS)

Ti-O # (line(2)) Name of the current curve: Coop/cohp for Ti-O which include Ti(3d, 4s,6p) and O(2s,2p)

Ti # (lines(3,20)) Reference atom, for which you could have included a list of atomic orbitals. Since there's none, all the orbitals of the Ti will be included in the analysis.

2.0 3.0 # (line(4)) Bond distance range in calculating COOP/COHP

O # (line(5)) Neighboring atoms, for which you could have included a list of atomic orbitals. Since there's none, all the orbitals of the O atoms in the range 2-3 Bohr will be included in the analysis.

Ti3d-O2s # Coop/Cohp for Ti(3d)-O(2s)

Ti_3d

2.0 3.0 # Bond distance range in calculating COOP/COHP

O_2s

Ti3d-O2p # Coop/Cohp for Ti(3d)-O(2p)

Ti_3d

2.0 3.0 # Bond distance range in calculating COOP/COHP

O_2p

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Then for COHP/COOP run the cammand in working directory :

$./mprop -s 0.1 -n 500 -m -25 -M 25 coo

Here -s parameter for energy smearing in calculate coop/cohp/pdos. It should be approximately equal to (M-m)/n, -n parameter is number of points in coop/cohp/pdos data -m and -M parameters is the lowest and highest energy

point for coop/cohp/pdos calculation. Remember there is no empty line in coo.mpr.

(b) For DOS/PDOS

make another text file entitled as *pdos.mpr* containing following :

BaTiO3 #outputname

DOS

Ti_dos

Ti

Ti3d

Ti_3d

Ti4s

Ti_4s

O2p

O_2p

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and use the cammond in working directory as :

$./mprop -s 0.01 -n 500 -m -15 -M 15 pdos

For details of this utility simply type "./mprop -h" in the COOP utility folder of SIESTA. It will give you the manual. Some test files are also given in ~/siesta/Util/COOP/Tests.

Now using a suitable plotting tool you can plot

*.PDOS, *.COOP or *.COHP files for different bonds.

All the best.

Please give the feedback in drmohanlv@gmail.com