# The complete Transiesta-Run

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These scripts have been prepared for complete transiesta run after series compilation of transiesta and tbtrans.

In order to compile transiesta in series Use following steps :

1. download siesta-trunk-462 from :

http://departments.icmab.es/leem/siesta/CodeAccess/Code/downloads.html

and extract it in home directory

now go to Obj dir and configure using :

$ /home/drmohanlv/siesta-trunk-462/Obj/ sh ../Src/obj_setup.sh

then

$ /home/drmohanlv/siesta-trunk-462/Obj/ ../Src/configure

finally compile transiesta using

$ /home/drmohanlv/siesta-trunk-462/Obj/ make transiesta

this will generate a "transiesta" binary file in this directory.

copy binary file to /home/drmohanlv/bin/ directory by

$ /home/drmohanlv/siesta-trunk-462/Obj/ cp transiesta ~/bin

now for compilation of tbtrans go to

$ /home/drmohanlv/siesta-trunk-462/Util/TBTrans_rep/

and only type make this will generate "tbtrans" binary file for further use

copy binary file to /home/drmohanlv/bin/ directory by

$ /home/drmohanlv/siesta-trunk-462/Obj/ cp tbtrans ~/bin

After above compilation of "transiesta" and "tbtrans" for transport properties studies follow the steps :

1-) Make the electrode input file elec.fdf for your system (don't change the name of file as well as system name).

2-) It should be notes that in ~/bin dir the binary/exe file of transiesta and tbtrans must be there.

3-) In presence of proper *.psf file for corresponding elements now run the first script for electrode using command

$ sh elec_script.sh

Your calculation should complete in a few minutes and will generate a elec.TSHS file.

4-) Plot the band structure with your own method.

5-) Now again modify *bias_script.sh* for your system and execute it using

$ sh bias_script.sh

6-) Next we need to run tbtrans for each bias steps. Modify tbtrans_script.sh and execute it.

$ sh tbtrans_script.sh

7-) When you finish the previous step, execute

$ sh get_IV_script.sh

This will genrate I-V values in I-V.dat file and you will have your I-V plot.

Tbtrans generates scat.AVTRANS file in each folder. First column is Energy, the second one is transmission, the third one is TotDOS and the last one is PDOS.

8-) In order to generate three data files in the corresponding directory for :

Energy vs Transmitance plot as EvsT.dat;

Energy vs Total density of states plot as EvsTD.dat and

Energy vs projected density of states plot as EvsPD.dat

you need to run one more script given in the same directory as getEvsX.sh which can be run using command :

$ sh getEvsX.sh

If you want to create data file containing required data for plot you can also use the fifth script i.e. copy-data-files.sh using

$ sh copy-data-files.sh

you can rename this data file as per the name of system and copy for further plotting.

If you find any problem with this example, feel free to inform/contact me in drmohanlv@gmail.com

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