Get a license for CALYPSO by going to this page and filling out the form.

Then download the latest CALYPSO package as well as the manual.

Install CALYPSO on your Linux/Mac machine using the instructions from the manual.

Make sure that Quantum ESPRESSO is installed and working correctly. Also make sure that you have the correct address to the 'pw.x' executable binary.

Now we can begin with the nanocluster global optimization.

You need to create 3 files.

First is the input.dat for CALYPSO. This should look like the following:

```
################################ The Basic Parameters of CALYPSO
################################
# A string of one or several words contain a descriptive name of the system (max. 40
characters).
SystemName = Z
# Number of different atomic species in the simulation.
NumberOfSpecies = 2
# Element symbols of the different chemical species.
NameOfAtoms = Zn S
# Number of atoms for each chemical species in one formula unit.
NumberOfAtoms = 3 3
# The range of formula unit per cell in your simulation.
NumberOfFormula = 1 1
# The volume per formula unit. Unit is in angstrom^3.
#Volume=60.0
# Minimal distance between atoms of each chemical species. Unit is in angstrom.
@DistanceOfIon
 1.0 1.0
 1.0 1.0
@End
# It determines which algorithm should be adopted in the simulation.
Ialgo = 2
# Ialgo = 1 for Global PSO
# Ialgo = 2 for Local PSO (default value)
# The proportion of the structures generated by PSO.
PsoRatio = 0.8
# The population size. Normally, it has a larger number for larger systems.
PopSize = 30
# It determines which local optimization method should be interfaced in the simulation.
ICode= 4
# ICode= 1 interfaced with VASP
# ICode= 2 interfaced with SIESTA
# ICode= 3 interfaced with GULP
# The number of lbest for local PSO
NumberOfLbest=4
# The Number of local optimization for each structure.
NumberOfLocalOptim= 1
# The precision of the K-point sampling for local optimization
Kgrid = 1 1
```

```
# The command to perform local optimiztion calculation (e.g., VASP, SIESTA) on your
computer.
Command = sh submit.sh
# The Max step for iteration
MaxStep =50
# If True, the metropolis rule is used during iterations
LMC= T
##########################End Basic Parameters ###################

###### The Parameters For Cluster structure prediction #########
# If True, a cluster structure prediction is performed.
Cluster= T
# The Vacancy length for 3 diminsional space
Vacancy = 15 15 15
####################End Cluster Parameters ######################
```

A file called ‘pw_input’ for Quantum ESPRESSO input.

```
&CONTROL
    calculation   = "relax"
    forc_conv_thr =  3.88938e-04
    max_seconds   =  6.22080e+08
    nstep         = 100
    pseudo_dir    = "/home/dmishra_du/Pseudopotentials/"
    outdir="temp"
    tprnfor       = .TRUE.
    tstress       = .TRUE.
/

&SYSTEM
    celldm(1)         = 1
!    a           =  2.00000e+01
    degauss     =  1.00000e-02
    ecutrho     =  4.40000e+02
    ecutwfc     =  5.50000e+01
    ibrav       = 0
    nat         = 6
    nbnd        = 50
    ntyp        = 2
    occupations = "fixed"
    smearing    = "gaussian"
/

&ELECTRONS
    conv_thr         =  1.00000e-06
    electron_maxstep = 200
    mixing_beta      =  7.00000e-01
    startingpot      = "atomic"
    startingwfc      = "atomic+random"
/

&IONS
    ion_dynamics = "bfgs"
/
```

```
ATOMIC_SPECIES
Zn      65.39000  Zn.pbe-van.UPF
S       32.06600  S.pbe-van_bm.UPF
```

A file called ‘submit.sh’ for CALYPSO:

```
#!/bin/sh
source compilervars.sh intel64
mpirun -np 8 '/home/dmishra_du/QE/qe-6.1/bin/pw.x' -inp pw_input> out.pw
```

Manas Sharma

I'm a physicist specializing in theoretical, computational and experimental condensed matter physics. I like to develop Physics related apps and softwares from time to time. Can code in most of the popular languages. Like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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