LASP Tutorial-1

LASP basic input/output files, lasp.in & lasp.str (alternatively, input & input.arc)

lasp.in

```
potential NN
explore_type sswoop
Ewaldflag    0
%block netinfo
  Co CoO.pot
  O  CoO.pot
%endblock netinfo
PrintChg 0

Run_type 15   #    12 for VC_DESW
              #    15 for SSW_crystal
              #    2  for DESW
              #    5  for SSW
              #    6  for ranMC_SSW
              #    16  for ranMC_SSW_crystal

SSW.SSWsteps  10000     # 0 single point
                        # 1 stru opt
                        # > 1  SSW global opt


#  for SSW search  start
SSW.Temp   100
SSW.NG           10
SSW.NG_cell      8
SSW.inirot   1
SSW.ftol        0.05
SSW.strtol   0.05
SSW.ds_atom 0.6
SSW.ds_cell 0.5

SSW.Ratio_Local                    15

SSW.output F
SSW.printevery F


SSW.LJcore      0

SSW.Safe_hardcurv      200
```

Free format； keywords； Case insensitive； Order insensitive

Keywords:

Potential **select Energy evaluation module**
support NN/VASP/SIESTA/LAMMPS/D3/US

Explore_type **select PES exploration/function module**
support
SSW/rigidssw/NVE/NVT/NPT/train

also see examples

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lasp.str: input coordinate

```
!BIOSYM archive 2
PBC=ON
                    Energy      5243          0.0433       -226.948405
!DATE
PBC     8.4709    5.6825   11.2059   90.0004   67.7928   89.9986
Co       5.865352171    3.542956874   10.341614008 CORE    1 Co Co    0.0000    1
Co       6.288756626    0.701772230    3.079438787 CORE    2 Co Co    0.0000    2
Co       3.747541522    0.701736357    5.154441268 CORE    3 Co Co    0.0000    3
Co       2.053402560    4.490091423    3.079723819 CORE    4 Co Co    0.0000    4
Co       4.170952429    1.648821996    8.267233490 CORE    5 Co Co    0.0000    5
Co       8.406643357    3.542883680    8.266704055 CORE    6 Co Co    0.0000    6
Co      11.371330527    4.489897261    9.304472195 CORE    7 Co Co    0.0000    7
Co       6.712327345    1.648772360    6.192408108 CORE    8 Co Co    0.0000    8
Co       9.677306957    0.701674982    7.229479027 CORE    9 Co Co    0.0000    9
O        7.551622523    4.489918211    9.813652366 CORE   30  O  O    0.0000   30
O        4.587096585    3.542863833    8.776603246 CORE   31  O  O    0.0000   31
O        0.774875744    4.490051678    1.513925691 CORE   32  O  O    0.0000   32
O        4.163232059    4.490009218    5.663787177 CORE   33  O  O    0.0000   33
O        2.469420179    0.701713885    3.589233130 CORE   34  O  O    0.0000   34
O        5.857769253    0.701651398    7.739090701 CORE   35  O  O    0.0000   35
O        6.704545848    4.490007896    3.588772315 CORE   36  O  O    0.0000   36
O        6.281438426    3.542973686    0.476852063 CORE   37  O  O    0.0000   37
end
end
```

follow .arc file format， by much simplified（e.g: The “CORE” information is not read after Line 6)

Line 1-4: information lines （see left figure for .arc）

Line 5 : heading by “PBC” Followed by lattice “a b c alpha beta gamma”

Line 6---end: Element name Cartesian coordinate x , y z

.arc file is a format utilized by Material Studio

End lines:
End
End

order insensitive

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Run a job

Prepare your files

For NN calculations, what you need is a NN potential file, *.pot

```
14:41:24:[zpliu@storage3 1]$ ll
total 352
-rw-rw-r-- 1 zpliu zpliu   3184 Jun  8 14:40 lasp.str
-rw-r--r-- 1 zpliu zpliu    741 Jun  8 14:41 lasp.in
-rw-r--r-- 1 zpliu zpliu 350212 Jun  8 14:41 CoO.pot
14:41:25:[zpliu@storage3 1]$ pwd
/home8/zpliu/CoOx/NN-test/1
```

SSW global optimization output

```
14:41:32:[zpliu@storage3 1]$ nohup mpirun -np 4 /home7/bin/lasp-release-1.0/lasp >out&
[1] 29956
14:43:59:[zpliu@storage3 1]$ nohup: ignoring input and redirecting stderr to stdout

14:43:59:[zpliu@storage3 1]$ ll
total 376
-rw-rw-r-- 1 zpliu zpliu   3184 Jun  8 14:40 lasp.str
-rw-r--r-- 1 zpliu zpliu    741 Jun  8 14:41 lasp.in
-rw-r--r-- 1 zpliu zpliu 350212 Jun  8 14:41 CoO.pot
-rw-rw-r-- 1 zpliu zpliu      0 Jun  8 14:43 out
-rw-rw-r-- 1 zpliu zpliu   3177 Jun  8 14:44 allkeys.log
-rw-rw-r-- 1 zpliu zpliu     25 Jun  8 14:44 best.arc
-rw-rw-r-- 1 zpliu zpliu     25 Jun  8 14:44 Badstr.arc
-rw-rw-r-- 1 zpliu zpliu     25 Jun  8 14:44 all.arc
-rw-rw-r-- 1 zpliu zpliu     60 Jun  8 14:44 SSWtraj
-rw-rw-r-- 1 zpliu zpliu   2744 Jun  8 14:44 lasp.out
```

lasp.out all text output

all.arc local minimum

SSWtraj Exothermic structures along trajectory

Best.arc Lowest energy structures along trajectory

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Other output files

allkeys.log all keywords (including the default values)

Badstr.arc The structures possibly predicted wrongly by NN calculation

When the keywords SSW.printevery T

There are another two files： they are important for NN fitting

allstr.arc output SSW trajectory structures

allfor.arc output force/stress corresponding to structure in allstr.arc

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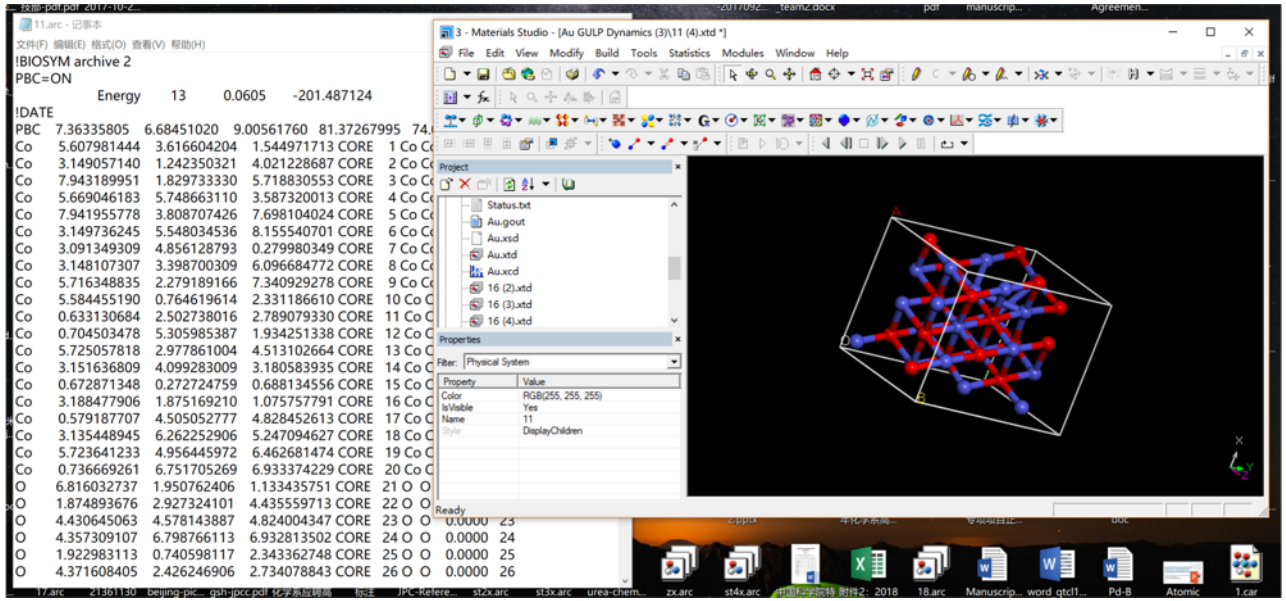
View results

View structures， including all.arc, best.arc, allstr.arc

Use Material Studio （WINDOWS system）to view all .arc file（animation）

Edit the file using notepad in windows



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View results in text

Lasp.out

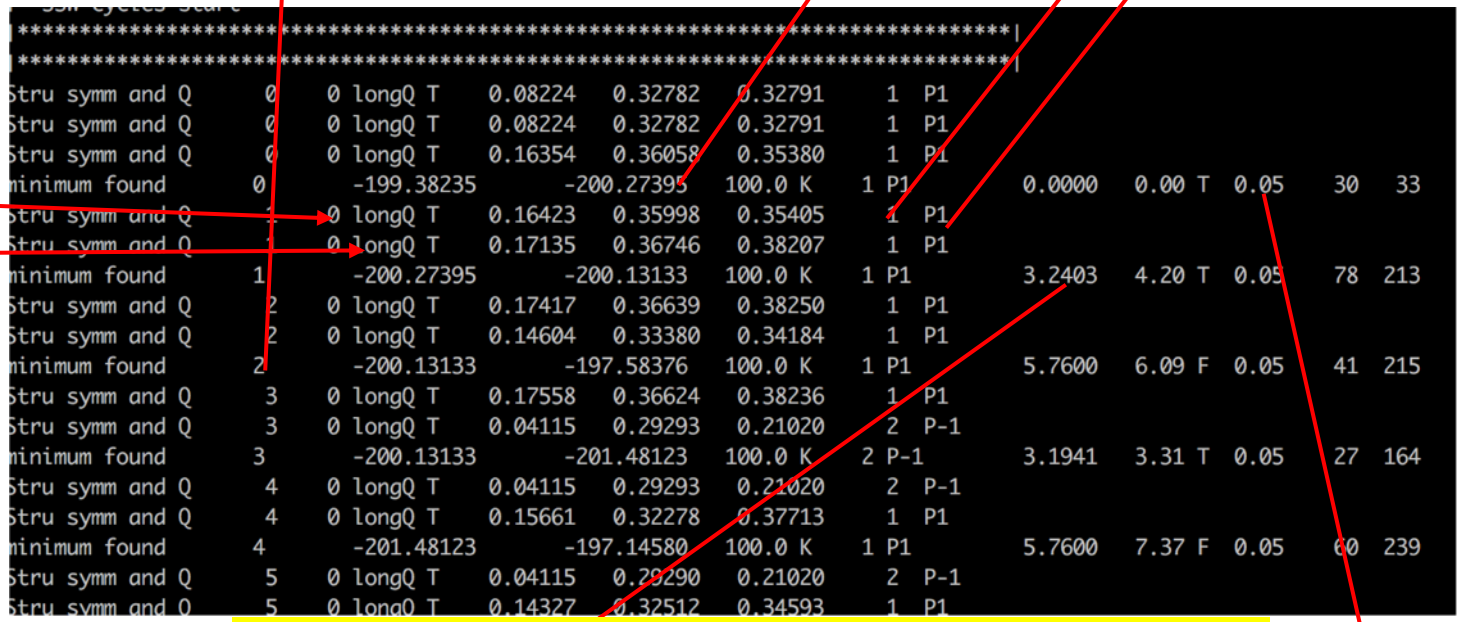
SSW steps

New minimum (energy)

New minimum space group

Order parameter for the initial and final state in one SSW

Order Parameter Q2 Q4 and Q6



Output example for SSW crystal structure exploration

Distance in SSW

Maximum force eV/Ang for new minimum

