NITheCS

National Institute for
Theoretical and Computational Sciences

NITheCS Mini-school

Wednesday 11, 18 and 25 May 2022, 14h00 – 15h00

Dr Kingsley Obodo (North-West University) and Dr Cecil Ouma (Next-Einstein forum fellow)

‘Quantum ESPRESSO’

Action plan 18th May 2022 Part 1

- Review/recap of the previous lesson (11th May 2022)
- Resources:
  a) Materialsproject{https://materialsproject.org/materials/mp-1094034/#}, Crystallography
  b) Open Database {https://www.iucr.org › resources› cif},
  c) http://rruff.geo.arizona.edu/AMS/minerals/Platinum,
  d) The Open Quantum Materials Database {https://oqmd.org/}, etc.
  e) BURAI works in windows,
  f) Materialscloud{https://www.materialscloud.org/work/tools/qeinputgenerator}, etc.
- Required optimizations:
  a) Lattice constant optimization,
  b) KPOINT optimization,
  c) ECUT optimization,
  d) Cell optimization.

Where to obtain atomic structures in CIF format

Covert from CIF to QE input format

Assignment

Resources

To obtain the structure

Generate the input files necessary for running on CHPC or a Linux system

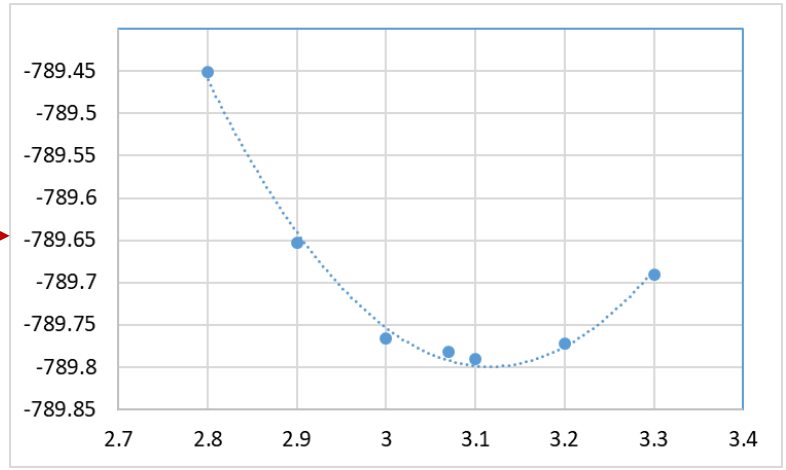
Running on CHPC

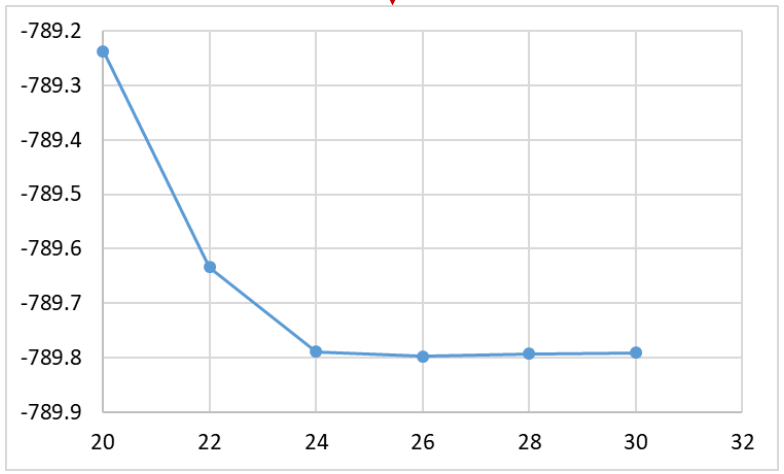
- ssh {username}@lengau.chpc.ac.za; where {username = studentXX, where XX = assigned number}
- cd to the /mnt/lustre/users/studentXX; calculations must be ran on /mnt/lustre

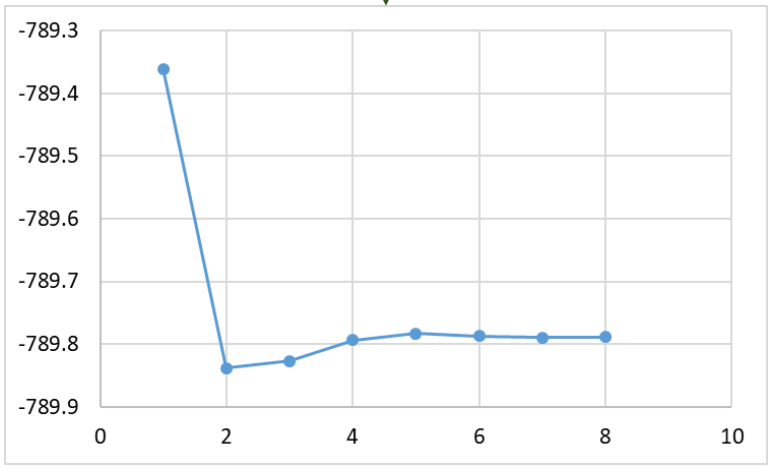
- The project name is WCHPC
- Number of nodes 1, wall time 04:00
- Enter email address
- Calculation type PW
- Click y to submit and n to review file before submission

Assignment result – Part 1

- Required optimizations:
  a) Lattice constant optimization,
  b) KPOINT optimization,
  c) ECUT optimization,
  d) Cell optimization.







For cell optimization, you need to change the calculation flag in the input file from 'scf' to 'vc-relax'

```
&CONTROL
  calculation = 'scf'
```

Tasks a) to c) can also be done via writing loop in bash script

Assignment result – Part 1 - Scripts

```
#!/bin/bash

PSEUDO=./pseudo

for a in 2.8 2.9 3.0 3.07 3.1 3.2 3.3 ; do

cat > Ti3C2_a$a.in << EOF
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   1.0000000000d-04
  forc_conv_thr =   1.0000000000d-04
  outdir = './temp_$a'
  prefix = '$a'
  pseudo_dir = '$PSEUDO'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
    a                   =  $a
    c                   =  1.51310e+01
    degauss             =  1.00000e-02
    ecutwfc             =  25
```

```
#!/bin/bash

PSEUDO=./pseudo

for c in 14.8 14.9 15.0 15.13 15.2 15.3; do

cat > Ti3C2_c$c.in << EOF
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   1.0000000000d-04
  forc_conv_thr =   1.0000000000d-04
  outdir = './temp_$c'
  prefix = '$c'
  pseudo_dir = '$PSEUDO'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
    a                   =  3.07064e+0
    c                   =  $c
    degauss             =  1.00000e-0
    ecutwfc             =  25
```

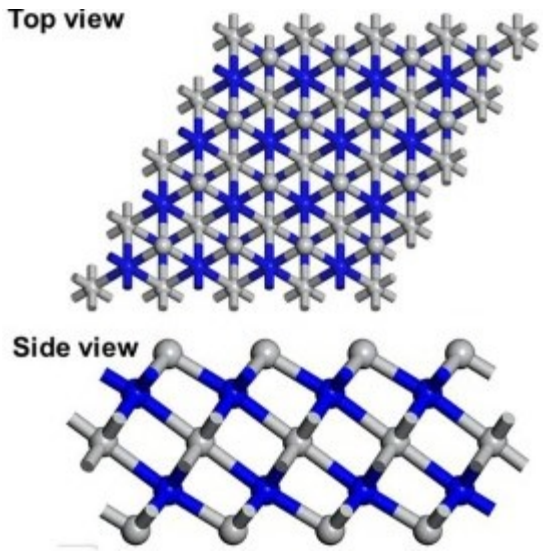
```
#!/bin/bash

PSEUDO=./pseudo

for K in 1 2 3 4 5 6 7 8; do

cat > Ti3C2_K$K.in << EOF
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   1.0000000000d-04
  forc_conv_thr =   1.0000000000d-04
  outdir = './temp_$K'
  prefix = '$K'
  pseudo_dir = '$PSEUDO'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
```

```
#!/bin/bash

PSEUDO=./pseudo

for ECUT in 20 22 24 26 28 30; do

cat > Ti3C2_E$ECUT.in << EOF
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   1.0000000000d-04
  forc_conv_thr =   1.0000000000d-04
  outdir = './temp_$ECUT'
  prefix = '$ECUT'
  pseudo_dir = '$PSEUDO'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
    a                   =  3.07064e+00
    c                   =  1.51310e+01
    degauss             =  1.00000e-02
    ecutwfc             =  $ECUT
```

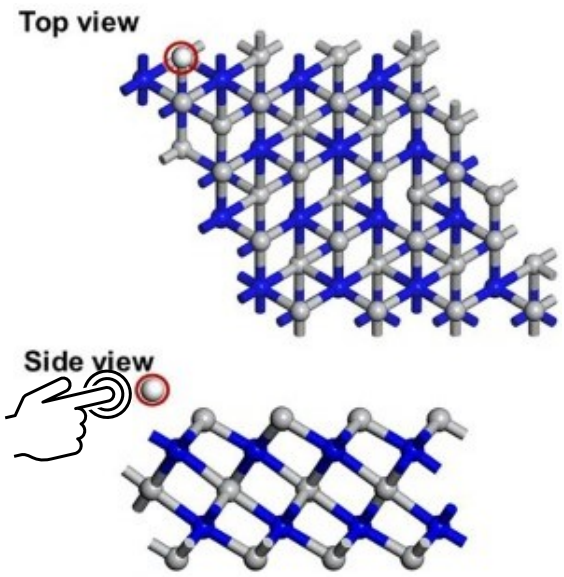
```
C           0.6666666700       0.3333333300       0.9141080000
C           0.3333333300       0.6666666700       0.4141080000
C           0.6666666700       0.3333333300       0.5858920000
C           0.3333333300       0.6666666700       0.0858920000
K_POINTS automatic
$K $K 1 0 0 0
```

Action plan 18th May 2022 Part 2

Case study hydrogen evolution reaction (HER) on Ti_3C_2 Mxene



Surface slab without H adsorbed



Surface slab with H adsorbed

- A hydrogen evolution reaction is the production of hydrogen through the process of water electrolysis.
- Hydrogen evolution usually occurs on metal electrodes
- Monitoring hydrogen evolution reactions is very important, since a redox reaction could take place during the process of corrosion of electrodes.

Action plan 18th May 2022 Part 2

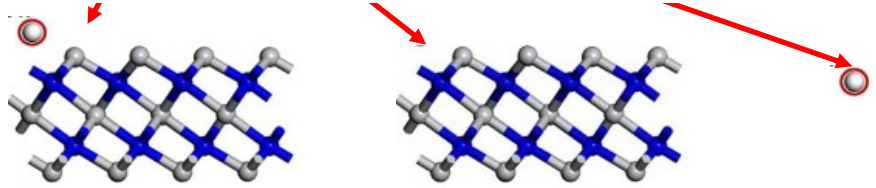
Case study hydrogen evolution reaction (HER) on Ti_3C_2 Mxene

Important equations

$$\Delta E_H = E_{S+H} - E_S - \tfrac{1}{2}H_{2(g)}$$

Hydrogen adsorption energy calculation

Total energies obtained from QE calculations



The expectations

System	Total energies from QE	This class: Unrelaxed	Assignment: Relaxed
Slab (S)	E_S	-3147.296	
Hydrogen (H)	E_H	-0.905	
S + H	E_{S+H}	-3148.512	
Adsorption energy	ΔE_H	-0.311	

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Ti_3C_2 unit cell = -786.82396029 Ry

Slab with H	Total energies (Ry)
Ti_3C_2_Htop	-3148.42644551
Ti3C2_HcenterofHextopofC	-3148.51153249
Ti3C2_HtopofC	-3148.50728737

Action plan 18th May 2022 Part 2

Case study hydrogen evolution reaction (HER) on Ti_3C_2 Mxene

Important equations

$$\Delta G_{\mathrm{H}} = \Delta E_H + \Delta E_{\mathrm{ZPE}} - T\Delta S_{\mathrm{H}}$$

Hydrogen adsorption energy calculation

Zero-point energy diff bet gaseous & adsorbed H

T = temp K and ΔS_H entropy change between adsorbed and gaseous species

The expectations

Optimal HER catalyst: $\Delta G \sim 0$ eV

Calculated ΔG = -4.23 eV

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