



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 11th May 2022

- Accessing Quantum espresso either via your own computer or the CHPC
- Structure files in CIF format obtained from either:
 - a) [Materialsproject](https://materialsproject.org/materials/mp-1094034/#){<https://materialsproject.org/materials/mp-1094034/#>}, Crystallography
 - b) Open Database {[https://www.iucr.org › resources › cif](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.
- Converting CIF to QE input file using either:
 - a) BURAI works in windows,
 - b) Materialscloud {<https://www.materialscloud.org/work/tools/qeinputgenerator>}, etc.
- Calculations intended:
 - Single point calculation (scf)
 - Lattice constant (relax)
 - Lattice constant and cell optimization (vc-relax)

Action plan 11th May 2022


- Require optimizations:
 - a) Lattice constant optimization (a, b & c),
 - b) KPOINT optimization,
 - c) ECUT optimization, Cell optimization.
- **Assignment:** Perform the band structure and density of states calculation on pristine Ti₃C₂bulk and monolayer. If you have any queries do not hesitate to contact me.
This we will work on in the next class.

Quantum ESPRESSO: The basics & download

- An integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.
- An **open-source** project
- Also referred to as PWSCF or QE
- What can QE do:
 - ❖ Ground-state calculations
 - ❖ Structural Optimization, molecular dynamics, potential energy surfaces
 - ❖ Electrochemistry and special boundary conditions
 - ❖ Response properties (DFPT)
 - ❖ Spectroscopic properties
 - ❖ Quantum Transport
 - ❖ Platforms

How to obtain QE

Step 1  <https://www.quantum-espresso.org/>



Step 2

home the project download users developers feats events news support us

download

To download the files you must be registered. If you are a registered user you can go directly to "download", otherwise please "register".

In order to download our free software and documentation, we kindly ask you to identify yourself through a nickname that you can obtain through a simple, non-intrusive, and strictly anonymous registration procedure. Once registered, you will not be asked any data for a second time.

Log In

nickname or e-mail password

☐ I'm not a robot

reCAPTCHA
Privacy - Terms

☐ remember me Step 3 download register | lost password

Quantum ESPRESSO: The basics & download

register

Would you mind telling something about yourself?

In order to keep providing the best open-source quantum simulation software available, to meet user expectations and the requests of our funding agencies, *we need to know a little bit about you for our files.*

The QUANTUM ESPRESSO Foundation is committed to your privacy. We do not request your name and the anonymous data that we collect will only be used to draft statistics about the number of (unique) downloads and the geographical, gender, and professional distribution of our users. This statistics may be published on this web site or used to write the reports that our public funding agencies request and to stir the future policies of the QUANTUM ESPRESSO Foundation and Project.

nickname *

email *

country *

--Select Country--

privacy policy *

☐ accept our privacy policy

[click to see our privacy policy](#)

Register

Step 3

register

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Thank you for registering. Click [HERE](#) to log in and download the files.

Step 4

download

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Log In

nickname or e-mail

Cecil

password

.....

☒ I'm not a robot



☒ remember me

download

[register](#)

[lost password](#)

Step 5

Quantum ESPRESSO: The basics & download

download

logout

SOFTWARE

DOCUMENTATION

OTHER

Full source code of QUANTUM ESPRESSO v7.0. Ready for compilation in all supported platforms. For more details and instructions see the release notes contained in the archive.

The full documentation bundle of QUANTUM ESPRESSO v7.0. Here you can find all the information on the features and capabilities of QUANTUM ESPRESSO.

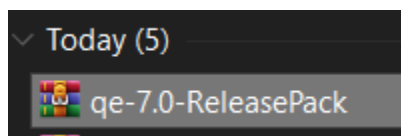
This archive contains the XSD schemas used by QUANTUM ESPRESSO applications in version 7.0. To download the package, press the button below.

Quantum ESPRESSO V.7.0

Quantum ESPRESSO V.7.0 Docs

Quantum ESPRESSO V.7.0 Schemas

Step 5



Instructions for the impatient:

```
cd qe-X.Y.Z/  
./configure  
make all
```

Other installations (Windows)

<https://burai.readthedocs.io/en/latest/install/download.html>

BURAI 1.3 documentation » Install »

Previous topic

Install

Next topic

Setting

Quick search

Go

Download

You can download executables from here:

- Windows
- Mac OSX
- Ubuntu

These zip-files contain precompiled executable files of Quantum ESPRESSO.

Step 1

Step 2

Step 3

BURAI 1.3 documentation » Install »

Setting

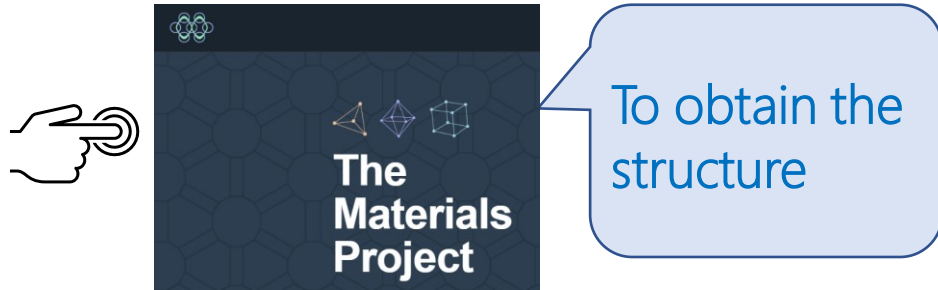
1. Unzip the downloaded file
2. Copy it to any directory on your computer e.g.:

- "C:\BURAI1.3_Windows" for Windows
- "/Applications/BURAI1.3.app" for Max OSX
- "/usr/share/applications/BURAI1.3" for Ubuntu

Step 4

Input file generation & Running on CHPC

NB: This tutorial will use Ti_3C_2 Mxene for all examples given

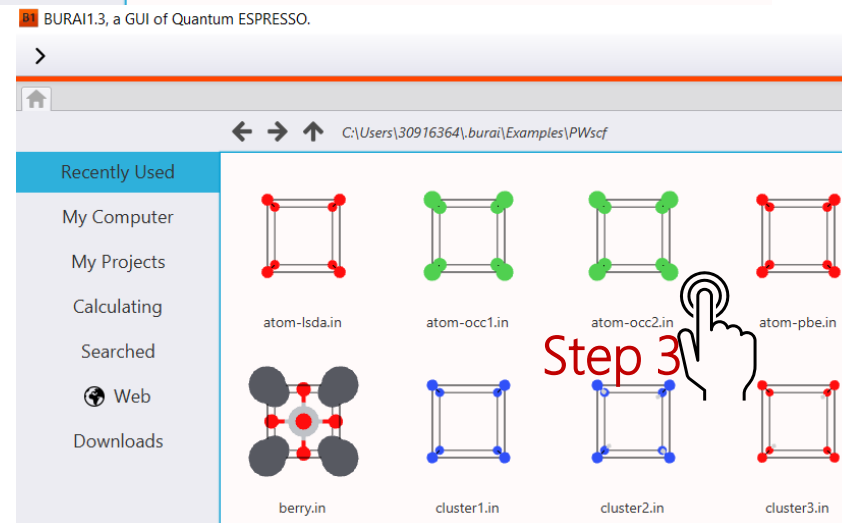
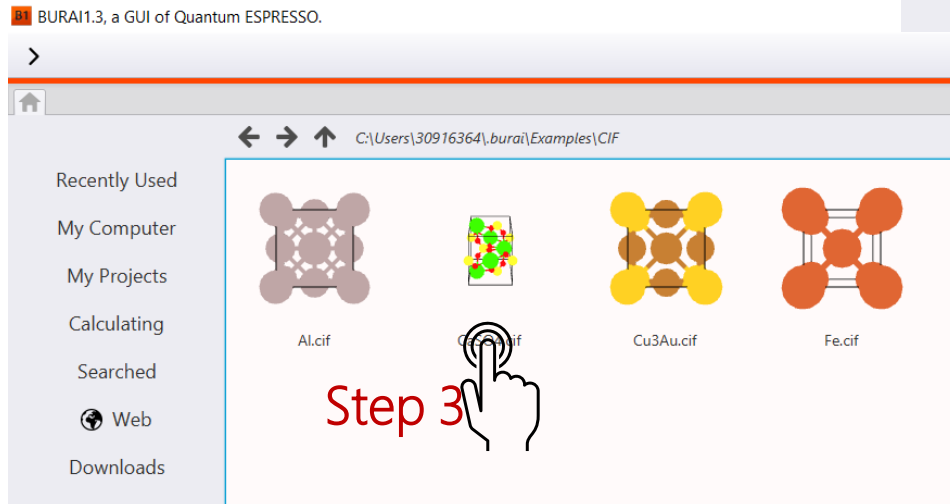
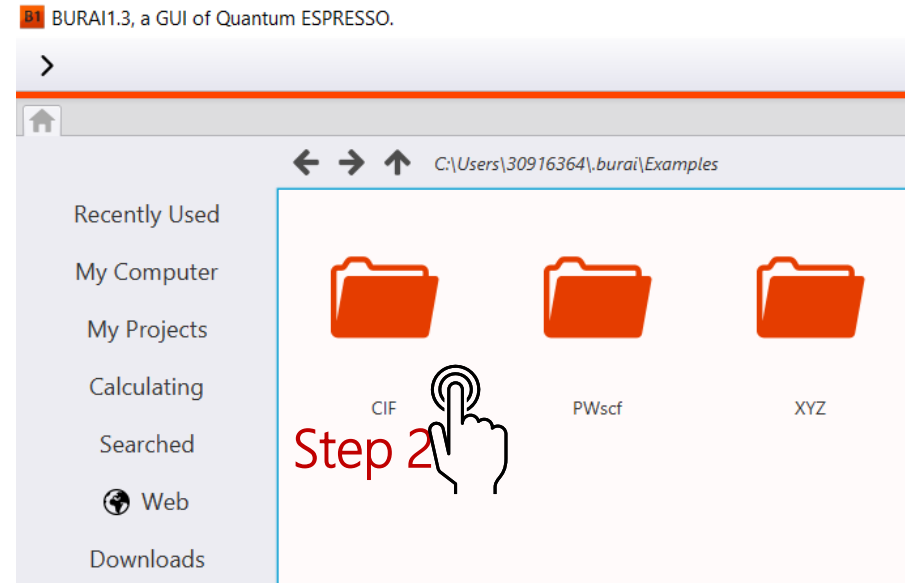
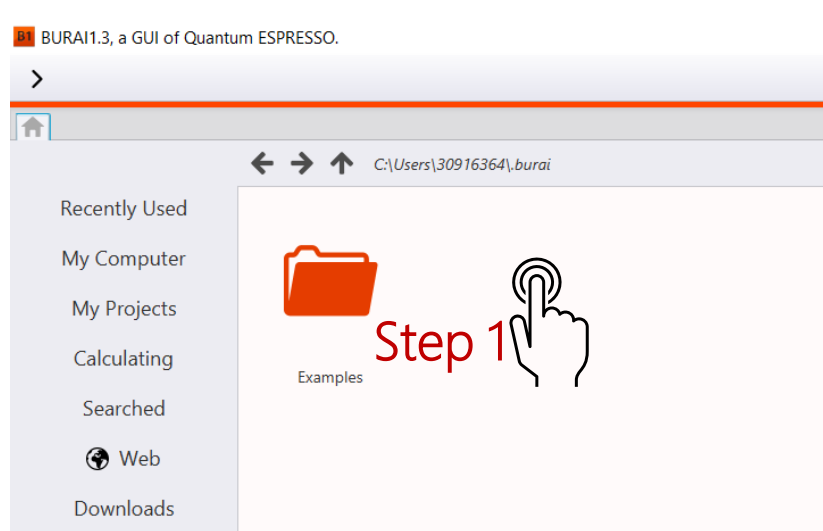


Run on CHPC

- `ssh {username}@lengau.chpc.ac.za`; where {username = studentXX, where XX = assigned number}
- `cd` to the `/mnt/lustre/users/studentXX` directory. All commands must be ran on `/mnt/lustre`
- To copy files from local computer to CHPC: `scp -r`
- We need a PBS submission script for this calculation, generate `qsub` script
- Enter `qesp_6.7` (tab to autocomplete).
- NOTE QE input file must end with `{NAME}.in`
- The project is on CHPC
- Number of nodes: all time 04:00
- Enter `qsub` command
- Check the job ID
- Check the job ID
- Submit job "qsub{filename}.pbs"
- Checking status of job "qstat-u \$USER"
- Cancelling job "qdel Job ID number"

Will be tacked later

Quantum ESPRESSO: Input file generation & visualization (BURAI)



Quantum ESPRESSO: Input file generation & visualization (BURAI)

The image displays the BURAI1.3 GUI for Quantum ESPRESSO. The main window shows a 3D visualization of a Ti3C2 molecular structure. The interface includes a sidebar on the left with icons for Result, Run, Screen-shot, Designer, Save as..., Save, Modeler, Input-file, and Show atoms. A 'Run a job' dialog box is open, allowing users to set conditions for a job, including Job Type (Optimize), Parallel settings (#Processes (MPI) 8, #Threads (OpenMP) 1), Host (Local Host), and Project (Save Project). The main window also features a 'Controlling Calculation' panel with settings for Restart Mode, Max Time, Max Steps, Variable Cell, Ion's Optimization (Threshold, Method), and Cell's Optimization (Threshold, Method, Pressure, Freedom). A red arrow points from the 'Optimize' button in the sidebar to the 'Run a job' dialog. Another red arrow points from the 'Optimize' button in the sidebar to the 'Optimize' button in the main window. A hand icon points to the 'Menu' button in the bottom left corner. A hand icon points to the 'Optimize' button in the bottom right corner. A hand icon points to the 'Dashboard' button in the bottom right corner.

Optimize

Run a job

Set conditions to run a job.

Job

Job Type: Optimize

Parallel

#Processes (MPI): 8

#Threads (OpenMP): 1

Host

Host Name: Local Host

Project

Save Project

Controlling Calculation

Restart Mode: no

Max Time: 1.72800e+05 sec

Max Steps: 1 51 101 151 201

Variable Cell: yes

Ion's Optimization

Threshold: 1.00000e-03 Ry/Bohr

Method: BFGS

Cell's Optimization

Threshold: 5.00000e-01 kbar

Method: BFGS

Pressure: kbar

Freedom: kbar

Menu

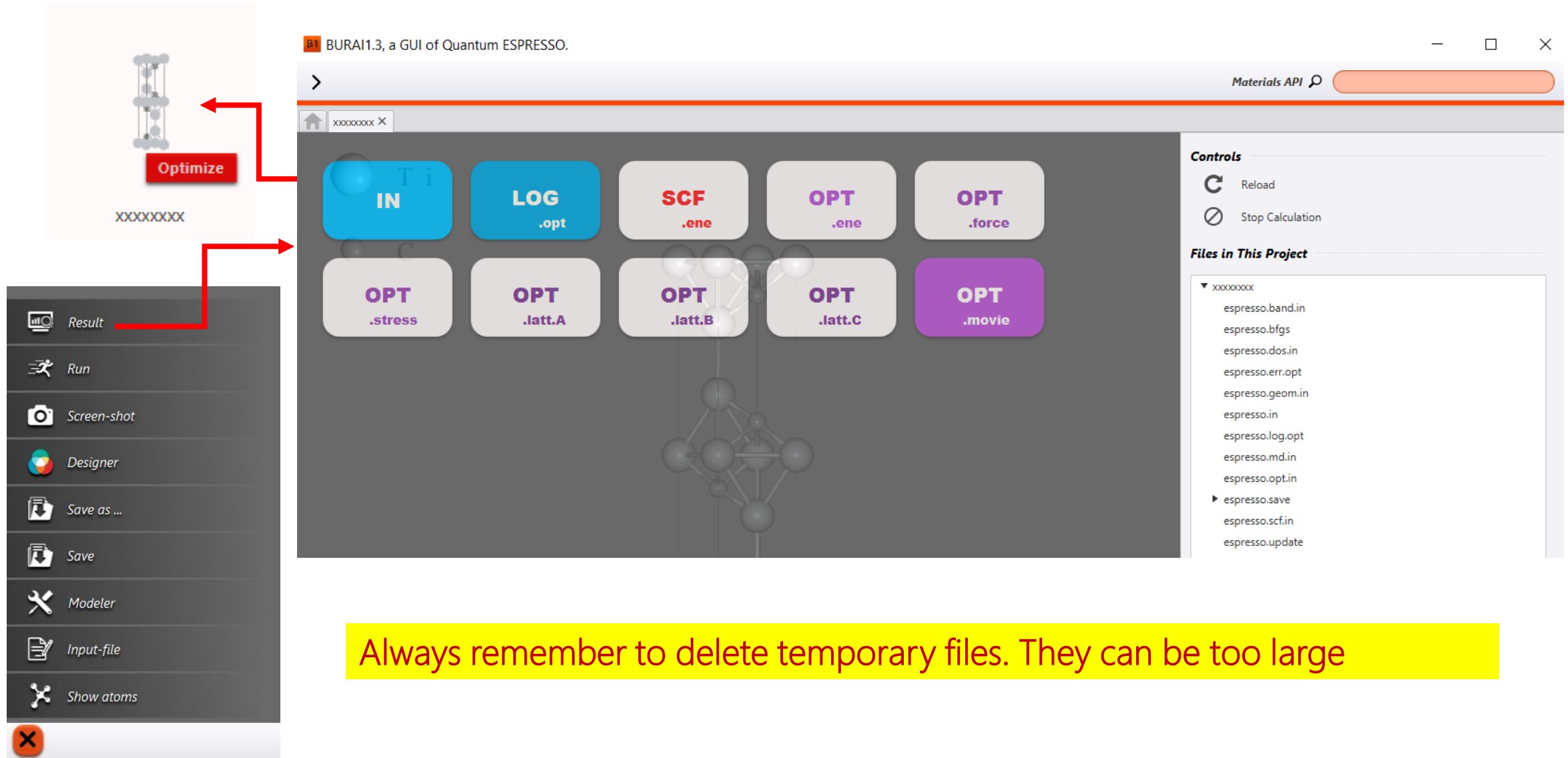
Dashboard

Optimize

Dashboard

NEB TD-DFT Geometry SCF Optimize MD DOS Band

Quantum ESPRESSO: Input file generation & visualization (BURAI)



The image displays the BURAI1.3 GUI, a tool for generating Quantum ESPRESSO input files. The main window features a grid of buttons for creating different file types: IN (blue), LOG (blue), SCF (red), OPT (purple), and OPT (purple). Below these are buttons for OPT (purple), OPT (purple), OPT (purple), OPT (purple), and OPT (purple). A sidebar on the left contains icons for Result, Run, Screen-shot, Designer, Save as ..., Save, Modeler, Input-file, and Show atoms. A top bar shows the title 'BURAI1.3, a GUI of Quantum ESPRESSO.' and a search bar labeled 'Materials API'. A right sidebar contains 'Controls' (Reload, Stop Calculation) and 'Files in This Project' (a list of files including espresso.band.in, espresso.bfgs, espresso.dos.in, espresso.err.opt, espresso.geom.in, espresso.in, espresso.log.opt, espresso.md.in, espresso.opt.in, espresso.save, espresso.scf.in, and espresso.update).

Optimize

XXXXXXXX

Result

Run

Screen-shot

Designer

Save as ...

Save

Modeler

Input-file

Show atoms

BURAI1.3, a GUI of Quantum ESPRESSO.

Materials API

XXXXXXXX

IN

LOG .opt

SCF .ene

OPT .ene

OPT .force

OPT .stress

OPT .latt.A

OPT .latt.B

OPT .latt.C

OPT .movie

Controls

Reload

Stop Calculation

Files in This Project

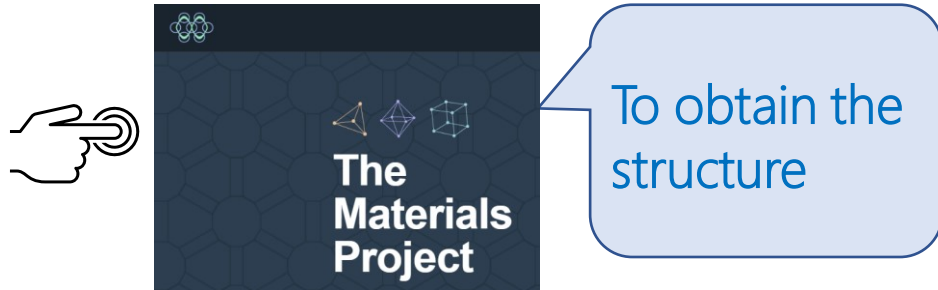
XXXXXXXX

- espresso.band.in
- espresso.bfgs
- espresso.dos.in
- espresso.err.opt
- espresso.geom.in
- espresso.in
- espresso.log.opt
- espresso.md.in
- espresso.opt.in
- espresso.save
- espresso.scf.in
- espresso.update

Always remember to delete temporary files. They can be too large

Input file generation & Running on CHPC

NB: This tutorial will use Ti₃C₂ Mxene for all examples given

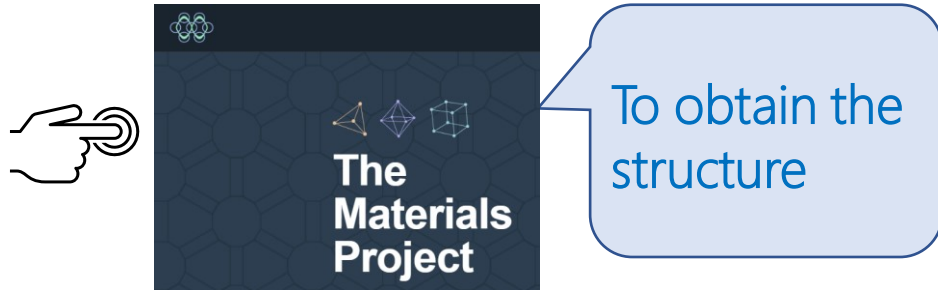


Run on own computer

- Then for scf, relax, vc-relax use the pw.x command.
- Open the input file using your favourite text editor, change calculation = 'scf' to 'relax' or 'vc-relax'.
- 'scf' does a single point calculation; 'relax' does atomic position relaxation, 'vc-relax' does full optimization.
- There are other type of calculations such as 'nscf', 'bands', etc.
- To run in serial, use `pw.x < {inputfilename} > {outputfilename} &`; with & calculation runs in the background
- To run in parallel use `mpirun -np 2 pw.x < {inputfilename} > {outputfilename}; -np` "Number of process" and the number can vary based on your computer.
- `ps -a` shows jobs running in the background.
- From the output file, the total energy can be read. The total energy is important to ensure structural minimization and calculation of other properties (to be discussed later).

Input file generation & Running on CHPC

NB: This tutorial will use Ti3C2 Mxene for all examples given



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`
- To copy files from local computer to the chpc: `scp-r`
- We need a PBS submission script to run this calculation, generate one as follows
- Enter `qesp_6.7` (tab key helps to autocomplete). NOTE QE input file should end with {NAME}.in
- 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
- Submitting job "`qsub{filename}.pbs`"
- Checking status of job "`qstat-u $USER`"
- Cancelling job "`qdelJob ID number`"