Quantum Espresso Tutorial

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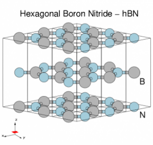
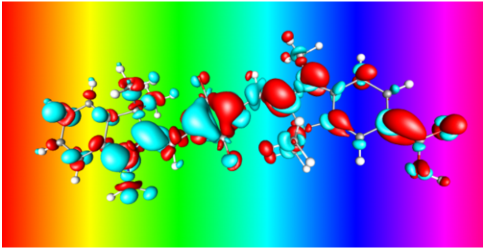


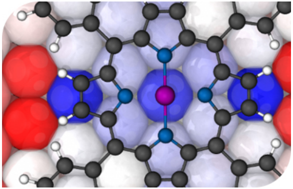
Quantum Espresso Tutorial : Background

- DFT is a very popular approach to materials modelling at the atomic scale.
- It strikes a balance between computational cost and accuracy.
- What can we compute with DFT?
  - Total energy
  - Band structure
  - Forces
  - Elastic properties
  - Phonons
  - Electric polarizability, Raman and infrared Activity
  - Electron-Phonon coupung, superconducting T_c



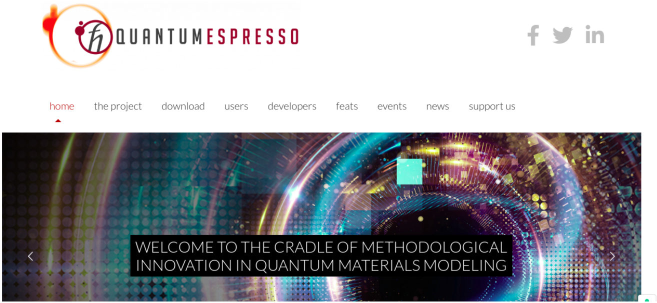
Quantum Espresso Tutorial : Background

- There are limits to DFT course, since its a ground state theory,
  - Time dependent properties
  - Localized *d* & *f* states
  - . . . ? hint:(**why are we here?**)



Quantum Espresso Tutorial: the code

- Quantum Espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the atomic scale
- It implements KS-DFT,
- Uses the Plane-wave and Pseudopotential method.



WELCOME TO THE CRADLE OF METHODOLOGICAL INNOVATION IN QUANTUM MATERIALS MODELING

Quantum Espresso Tutorial: the distribution

- The code can be obtained freely from the QE website,
- Development versions are at: [https://gitlab.com/QEF/q-e/tags]

- The code is FOSS, community contributions.
- [https://www.quantum-espresso.org/manifesto/]

Quantum Espresso Tutorial: Packages

- Since its a suite of integrated codes, what are they?
  - pw.x SCF, NSCF, Force minimization,
  - dos.x Density of states (post processing)
  - bands.x Band structure
  - ph.x DFPT
  - neb.x reaction pathways
  - atomic.x atomic calculations

QUANTUMESPRESSO

Quantum Espresso Tutorial: Packages and plugins

- Advanced
  - gipaw
  - WanT a plugin
  - Plumed

Quantum Espresso Tutorial: Outputs

- What can QE do?
  - Ground state calculations
  - Structural optimization, MD,
  - Electrochemistry and special boundary conditions
  - Response properties (DFPT)
  - ...
- Full list: [https://www.quantum-espresso.org/what-can-qe-do/]

Quantum Espresso Tutorial: Installing

- QE provide a standard approach to compiling and installing the code

```
./configure
make pw pp
make install
```

- You of course need to have the prerequisites, such as a **compiler**, **FFTW library**, **LAPACK/BLAS**. . .
- We wont need to do the installation for the tutorial, this has been done for you.

Quantum Espresso Tutorial: Running a Calculation

- The code's executable are run from a typical shell environement,

```
~$ pw.x <scf_input.in>  scf_output.out
```

- It requires some preparation ahead of time
  - choosing pseudopotentials
  - the structure
  - input parameters . . .

Quantum Espresso Tutorial: Input Documentation

- The executable in QE will read data from an input file:

```
~$ pw.x < scf_input.in
```

- The file has a very specific structure:

```
&NAMELIST1 ... /
&NAMELIST2 ... /
&NAMELIST3 ... /
&INPUT_CARD1
...
&INPUT_CARD2
...
...
```

Quantum Espresso Tutorial: Input Documentation

- **NAMELIST** are standard input constructs in F90
- They allow the specification of a value for an input variable when needed, and defaults otherwise.
- The variables inside the nameslist can appear in any order.

```
&NAMELIST
   example_variable2=XX,
   example_variable1=YY
   ...
```

- **NAMELISTS** are read in a specific order.
- **NAMELISTS** that are not required are ignored.

Quantum Espresso Tutorial: Input Documentation

- **INPUT_CARDS** are specific to Quantum Espresso,
- They provide a means to specify data that is required, and is inconvenient to put in using NAMELIST format
- **INPUT_CARDS** Requires that data is in a specific order,

```
INPUT_CARDS  card_format_specifier
data(1,1) data(1,2) data(1,3)...
```

Quantum Espresso Tutorial: Input Documentation

- **Mandatory NAMELISTS** In Quantum Espreso are these three:

```
&CONTROL Input variables that control the calculation and the amount of I/O on disk and the screen
```

```
&SYSTEM  input variables that specify the system  under study
```

```
&ELECTRON  input variables that control the algorithms used to reach self-consisten solution of KS equation for the electrons
```

Quantum Espresso Tutorial: Input Documentation

- **Mandatory** **INPUT_CARDS** In Quantum Espreso are three:

```
ATOMIC_SPECIES  name, mass and pseudos for each species present
```

```
ATOMIC_POSITIONS  type and coordinates of each atom in the unit cell
```

```
K_POINTS  coordinates and weights of the k-points used for BZ
     integration
```

Quantum Espresso Tutorial: Understanding the calculation

- **Energy Cutoff**: controls the number of basis functions used to espand the wave function
- **Pseudopotential**: a modification of the ionic potential which allows one to greatly reduce the number of plane waves needed without changing the chemical properties of the atoms.
- **BZ sampling** we have to sample over the first BZ with a discrete grid.

Quantum Espresso Tutorial: Silicon Hands On Example

- We can run the Silicon example,
- Copy the files to your home directory and work from there:

```
~$ cp -r /media/ictpuser/smr3694/ictptutor/YAMBO_TUTORIALS .
~$ cd YAMBO_TUTORIALS/Silicon/PWSCF
```

- Follow the Tutorial on the Yambo Wiki: Click this [https://www.yambo-code.eu/wiki/index.php?title=Silicon]

Quantum Espresso Tutorial: Silicon Hands On Example

- Great,
- We will have a break before we do the next step,
- Learning to generate Yambo Inputs.

Generating Yambo Databases from PWSCF

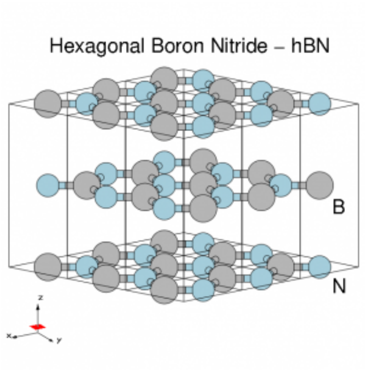
- We will use **Quantum Espresso** to generate KS-DFT eigenvalues and WFs,
- It implements **KS-DFT**, among other things.
- Freely available (FOSS).
- Yambo uses the results of your PWSCF calculations as the starting point.
- You need to be able to run SCF+NSCF calculations before getting to G0W0 with yambo.
- we will follow the bulk h-BN tutorial on the Yambo Wiki [https://www.yambo-code.eu/wiki/index.php/Bulk_material:_h-BN]

Prerequisites

- **Quantum Espresso**, it is installed on the ICTP machines.
- Input files and pseudopotentials : please copy them from the tutor directory.
- yambo: provides p2y, this is installed on the ICTP machines.

The System

- Bulk hBN is a HCP structured nitride,
- Four atoms per cell, 16 electrons in the unit cell,
- Lattice constants: a=4.176$a.u.$,c/a=2.582



Loggin In to Your ICTP Machine,

- Over **SSH**:

```
~$ ssh -i .ssh/smryambo  ictpuser@insXXXX...it
```

- where XXXX is a number, this should have been sent to you.
- Over the **browser** chrome/firefox/safari: https://insXXXXX.ictp.it
- enter the provided password.

Running Quantum espresso

- **Spack** commands will be used to load the environement to have access to the pwscf executable, and later p2y

```
~$ spack load quantum-espresso
~$ spack load yambo
```

Retreving the files:

- Copy the files to your home directory and work from there:

```
~$ cp -r /media/ictpuser/smr3694/ictptutor/YAMBO_TUTORIALS .
~$ cd YAMBO_TUTORIALS/hBN/PWSCF
```

DFT Calculations

- From the **PWSCF** directory, you will observe that you have the following:

```
Inputs
Pseudos
References
hBN_2D_nscf.in
hBN_2D_scf.in
```

- These are the required files for this exercise.

Executing the steps

- Run the SCF and NSCF steps:

```
~$ mpirun -np 2 pw.x < hBN_scf.in > hBN_scf.out
```

- The SCF generates the ground state $n(r)$, occupations, Fermi level...

```
~$ mpirun -np 2 pw.x < hBN_nscf.in > hBN_nscf.out
```

- The NSCF calculation will compute the KS eigenvalues and eigenvectors for all the requested **nbnd**

DFT Calculations

- Some important entries in the **PWSCF** input file:

```
wf_collect=.true.
force_symmorphic=.true.
diago_thr_init=5.0e-6,
diago_full_acc=.true.
```

- These are needed by yambo, see the wiki for more, and the QE documentation for more,

QUANTUMESPRESSO

What do we have?

- **PWSCF** creates a **hBN.save** dir,
- This is where we will work from for the next task.

```
ls hBN.save/
B.pz-vbc.UPF  charge-density.dat    wfc1.dat   wfc11.dat  wfc13.dat
      wfc2.dat  wfc4.dat  wfc6.dat  wfc8.dat
N.pz-vbc.UPF  data-file-schema.xml  wfc10.dat  wfc12.dat  wfc14.dat
      wfc3.dat  wfc5.dat  wfc7.dat  wfc9.dat
```

Conversion to Yambo Format: P2Y

- Yambo provides the **p2y** executable that can converd **PWSCF** outputs to **YAMBO databases**.
- It requires no input specific input file. . .
- How to do that:

```
$ cd hBN.save/
$ p2y
...
...
 <---> == DB3 (PseudoPotential) ... done ==
 <--->  == P2Y completed ==
$
```

SAVE Directory

- **p2y** generates a **SAVE** directory

```
$ ls
B.pz-vbc.UPF  SAVE                    data-file-schema.xml  wfc10.dat
     ....
$ ls SAVE
ns.db1                           ns.kb_pp_pwscf_fragment_13  ns.
     kb_pp_pwscf_fragment_6  ns.wf_fragments_11_1  ns.
     wf_fragments_3_1  ...
```

- What are these files?

yambo -D

- The **n*** files are netCDF formated files, you need to use the yambo -D command to check the information they hold:

```
$ yambo -D

[RD./SAVE//ns.db1]-------------------------------------------------------------
 Bands                                            :   100
 K-points                                         :   14
 G-vectors                                        :    8029 [RL space]
...
...
[RD./SAVE//ns.kb_pp_pwscf]-----------------------------------------------------
 Fragmentation                                    : yes
- S/N 004626 --------------------------------------------- v.05.01.00 r.21422
$
```

What next?

- The convention for moving from here, is usually to take the **SAVE** directory somewhere else, where you will proceed with the rest of the G0W0 calculations

P2Y advanced usage

- If you need to know more about how P2Y can be used, refer to this page on the wiki: Conversion to Yambo Format

Next

- You now have the neccessary inputs for G0W0 and more
- Before doing the G0W0 runlevel, you need to initialize first
- Then generate an input
- This will be done in the first G0W0 exercise

Thanks

- This is as much as we need for the **PWSCF** tutorial.
- Thank you!

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