# Introduction to YamboPy

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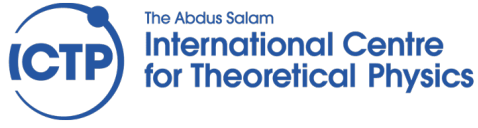



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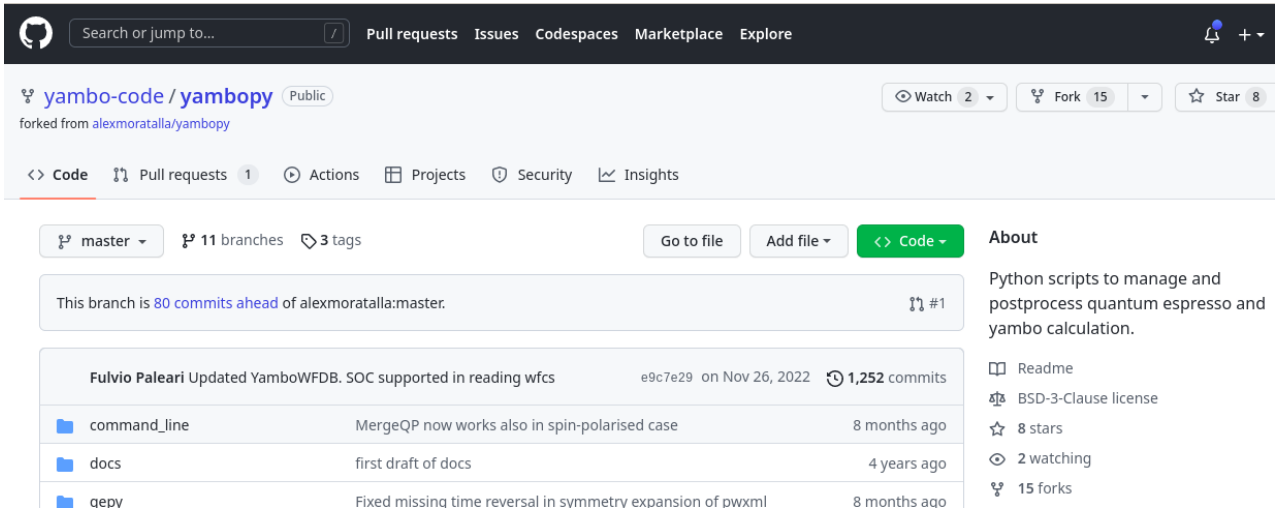
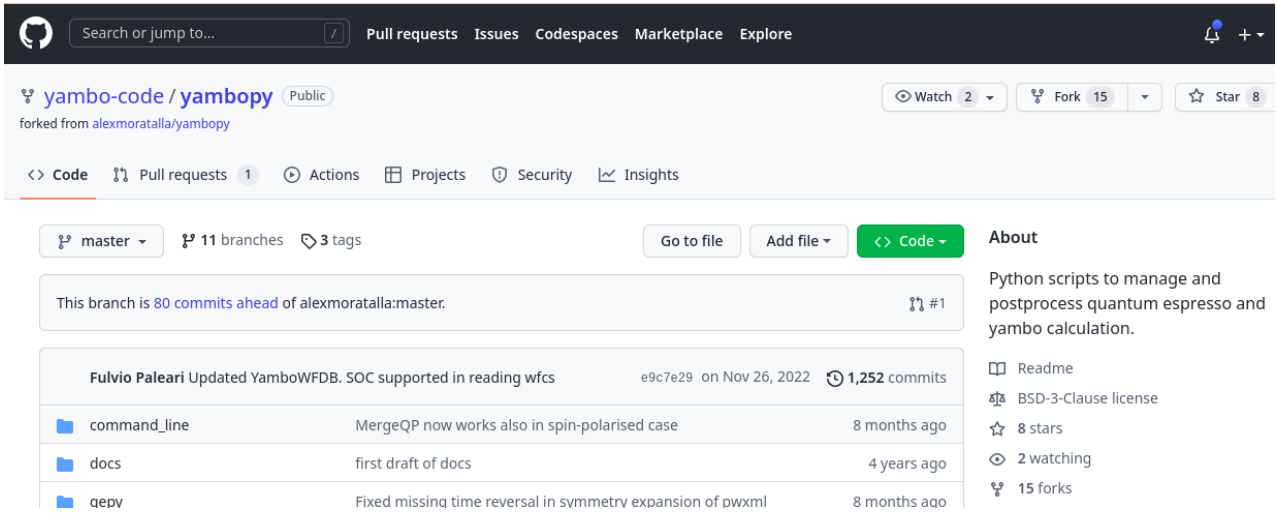
# Yambopy

- This project provides python scripts to manage and postprocess quantum espresso and yambo calculation.
- Can automate your calculations,
- provide post-processing capabilities
- Visualization
- Input file manipulation, etc.
- Its FOSS! https://github.com/yambo-code/yambopy



# Why?

- Automation reduces **mistakes**.
- Increase the **pace** of your work.
- **High Througput** studies.
- Key: **reproducibility**, can we achieve this?



# Requirements

- These python scripts require **python3**
- We will need:
  1. **yambopy**, Already Installed
  2. **yambo**, Installed
  3. **Quantum Espresso**, installed


# Aims of this Exercise:

- We will work on the Convergences and Approximations tutorial: click here
- And the database tutorial: click here
- Finally the BSE exercise: Click here

# Retreving the files:

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

```
~$ cp -r /media/ictpuser/smr3694/ictptutor/yambopy/tutorial ~/
    tutorial
~$ cd ~/tutorial
```

# Getting started

- You have to use spack to get the environment that provides yambopy:

```
~$ spack load quantum-espresso
~$ spack load yambo
~$ spack load anaconda3
```

# Running yambopy:

- First exercise,

```
~$ cd ~tutorial/run_calculations
~$ python gs_bn.py -sn
...
```

- Follow the steps here: click this
- You will run QE followed by GW convergence

# Analysis:

- Yambopy provides the capability to read and analyze the yambo NetCDF databases, for this exercise, start from this directory:

```
~$ cd ~tutorial/databases_yambopy
~$ yambopy save -nscf BSE_saves/QE_saves/hBN.save
...
```

- Continue with the tutorial: click here

# BSE with Yambopy

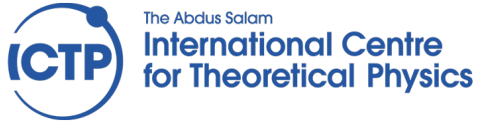
- This requires the first exercise to have been done
- We continue from the first exercise's directory:

```
1 ~$ cd ~tutorial/run_calculations
2 ~$
3 ...
```

- Continue with the instructions here: click this

# Thanks

- Thank you for your attention.
- questions?



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