

# Introduction to YamboPy

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CNR  
Istituito di Struttura  
della Materia



# 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>

The screenshot shows the GitHub repository page for `yambo-code/yambopy`. The repository is public and has 15 forks and 8 stars. It is forked from `alexmorata/yambopy`. The page shows the `master` branch with 11 branches and 3 tags. The repository is 80 commits ahead of `alexmorata:master`. The commit history shows a recent update by Fulvio Paleari on Nov 26, 2022, with 1,252 commits. The repository contains three folders: `command_line`, `docs`, and `oeov`. The `command_line` folder has a commit from 8 months ago with the message "MergeQP now works also in spin-polarised case". The `docs` folder has a commit from 4 years ago with the message "first draft of docs". The `oeov` folder has a commit from 8 months ago with the message "Fixed missino time reversal in symmetry expansion of oewxml". The repository is licensed under the BSD-3-Clause license and has 2 watchers and 15 forks.

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yambo-code / yambopy Public Watch 2 Fork 15 Star 8  
forked from alexmorata/yambopy

<> Code Pull requests 1 Actions Projects Security Insights

master 11 branches 3 tags Go to file Add file Code About

This branch is 80 commits ahead of alexmorata:master #1

Fulvio Paleari Updated YambopyFDB. SOC supported in reading wfcs e9c7e29 on Nov 26, 2022 1,252 commits

command_line	MergeQP now works also in spin-polarised case	8 months ago
docs	first draft of docs	4 years ago
oeov	Fixed missino time reversal in symmetry expansion of oewxml	8 months ago

Readme  
BSD-3-Clause license  
8 stars  
2 watching  
15 forks

# Why?

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

The screenshot shows the GitHub repository page for yambo-code/yambopy. At the top, there is a search bar and navigation links for Pull requests, Issues, Codespaces, Marketplace, and Explore. The repository name is yambo-code / yambopy, with a 'Public' label and statistics for Watch (2), Fork (15), and Star (8). Below this, there are tabs for Code, Pull requests (1), Actions, Projects, Security, and Insights. The main content area shows the current branch as master, with 11 branches and 3 tags. A message indicates the branch is 80 commits ahead of alexmorata/alexmorata:master. A commit by Fulvio Paleari is highlighted, titled 'Updated YamboWFBDB. SOC supported in reading wfcs', dated Nov 26, 2022, with 1,252 commits. Below the commit, a table lists files: command\_line (MergeQP now works also in spin-polarised case, 8 months ago), docs (first draft of docs, 4 years ago), and oev (Fixed missing time reversal in symmetry expansion of oev.xml, 8 months ago). On the right, the 'About' section describes the repository as Python scripts for managing and postprocessing quantum espresso and yambo calculations, and lists metadata like Readme, BSD-3-Clause license, 8 stars, 2 watchers, and 15 forks.

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command_line	MergeQP now works also in spin-polarised case	8 months ago
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Python scripts to manage and postprocess quantum espresso and yambo calculation.

Readme BSD-3-Clause license 8 stars 2 watching 15 forks

# 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](#)



## Retreiving the files:

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

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



# Getting started

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

```
1 ~$ spack load quantum-espresso  
2 ~$ spack load yambo  
3 ~$ spack load anaconda3
```



# Running yambopy:

- ▶ First exercise,

```
1 ~$ cd ~tutorial/run_calculations
2 ~$ python gs_bn.py -sn
3 ...
```

- ▶ 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:

```
1 ~$ cd ~tutorial/databases_yambopy
2 ~$ yambopy save -nscf BSE_saves/QE_saves/hBN.save
3 ...
```

- ▶ Continue with the tutorial: [click here](#)



# BSE with Yambo

- ▶ 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?

