

# QESG (Quantum ESPRESSO Script Generator)

*This programme is not a part of Quantum ESPRESSO official distribution.*

## 1 Required files

- **main.cpp**: main file including window\_main.h
- **window\_main.h**: header file defining "window\_main" class
- **window\_main.cpp**: file containing implementation of class "window\_main"
- **add\_atomic\_pos.h**: header file defining "add\_atomic\_pos\_window" class
- **add\_atomic\_pos.cpp**: file containing implementation of class "add\_atomic\_pos\_window"
- **basic\_script.in**: file containing text for script\_buffer (updated after using "Set basic script" option)
- **basic\_script\_old.in**: file containing previous text for script\_buffer (updated after using "Set basic script" option)
- **basic\_script.txt**: text file containing proposed and default basic script (enables setting back the default script text)
- **temp\_script.in**: file containing script with latest changes (e.g. in case of program error)

## 2 Compiling, libraries and usage

This programme was created, compiled and tested on GNU/Linux platform. To compile program use command:

```
g++ main.cpp -o main 'pkg-config gtkmm-3.0 --cflags --libs'
```

According to official site:

*Before attempting to install gtkmm 3.0, you might first need to install these other packages.*

- *libsic++ 2.0*
- *GTK+ 3.0*
- *glibmm*
- *cairomm*
- *pangomm*
- *atkmm*

Further information can be found at:

<https://developer.gnome.org/gtkmm-tutorial/unstable/sec-installation-dependencies.html.en>

The recommended way to use the program is to use "basic\_text.txt" as basic script. Any option that is not included in the program can be added manually in the script tab. This program is just a script generator. It does not check for bugs in script and is recommended for skilled users of quantum espresso.