

User guide for pqe

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Abstract. Please email me if there exist some bugs.

1. Installation instruction

The package of p can be obtained from the github website:

[https : //github.com/XVDing/pqe](https://github.com/XVDing/pqe)

First: uncompressing the pqe-pqe.zip file, then go into the uncompressed file.

Second: find the pqe file. Editing this file and modifying the file_path variable to the current path. (eg. file_path="/home/dxy/software/QE/pqe") .

Third: Entitle the pqe executable authority: chmod +x pqe

Fourth: Add the path for pqe to the ~/.bashrc file.

(eg. export PATH=/home/dxy/software/QE/pqe:\$PATH).

Note That: the path /home/dxy/software/pvasp above should change to your own file path of the location for pvasp executable file.

2. Introduction

pqe is a pre- and post-processing software for Quantum Espresso calculation.