winmostar tutorial

Quantum ESPRESSO BoltzTraP

V11.2.4

18 Oct. 2022 X-Ability Co., Ltd.

About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
-

Overview

- Using Quantum ESPRESSO (hereafter referred to as QE), we perform an NSCF calculation for the Mg_2Si crystal to obtain the total density of states.Based on the output files from QE, we then use BoltzTraP to calculate transport coefficients by solving the Boltzmann transport equations.

Note :

- The choice of k-points, type of pseudopotential, and cutoff energy can impact the calculation results.

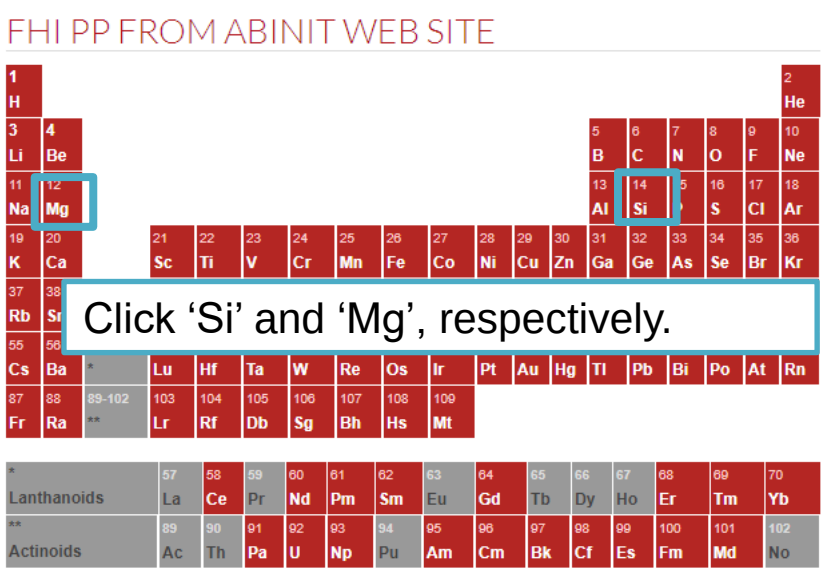
Preference of Operating Environment

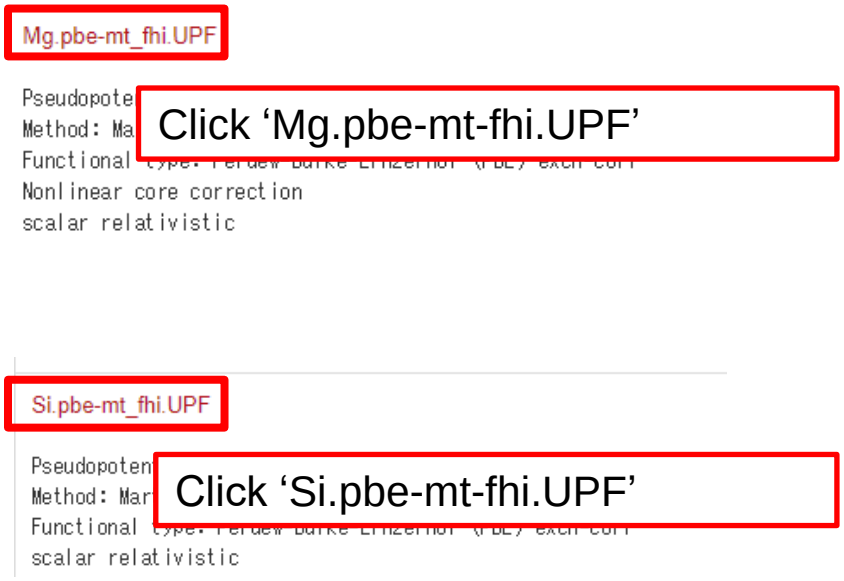
- For users of Winmostar version V11.5.0 or later on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version after 2023/04/05 includes the recommended version of 64-bit Quantum ESPRESSO.

- If the above does not apply to you or if you wish to use a version of Quantum ESPRESSO other than the recommended one, you will need to install and configure Windows version of Quantum ESPRESSO separately.

Download and Register Pseudopotentials

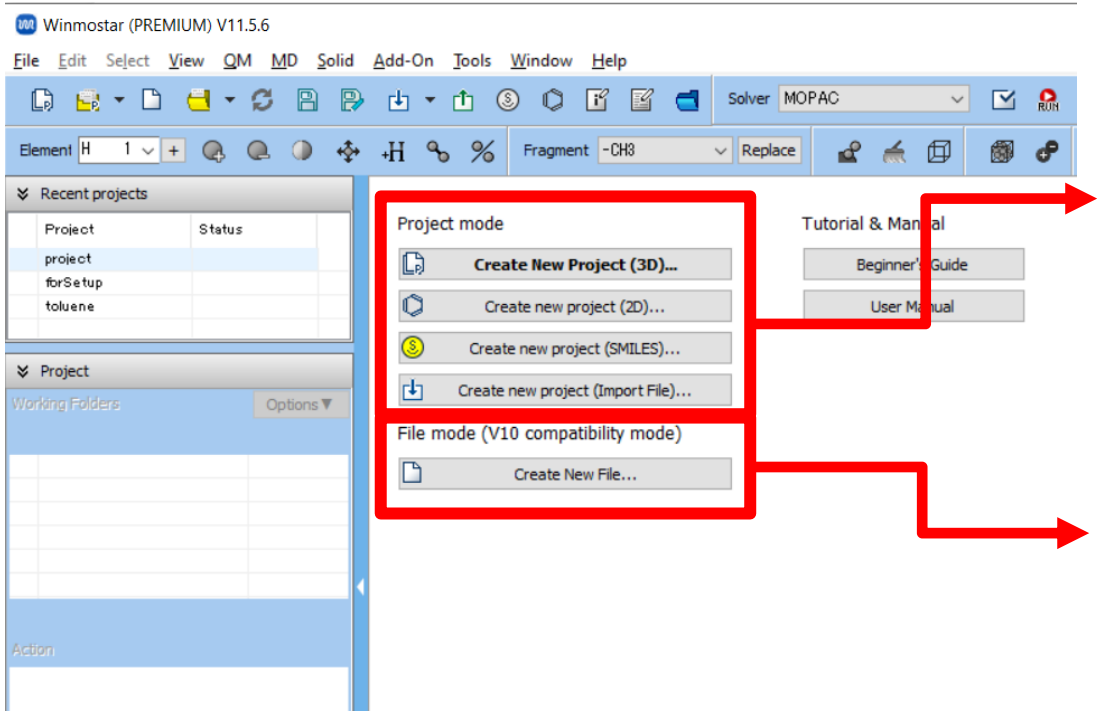
Download Si.pbe-mt-fhi.UPF and Mg.pbe-mt-fhi.UPF from the URL below,
place them in the pseudo folder located under your Quantum ESPRESSO installation directory,
and then restart Winmostar.
http://pseudopotentials.quantum-espresso.org/legacy_tables/fhi-pp-from-abinit-web-site





Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

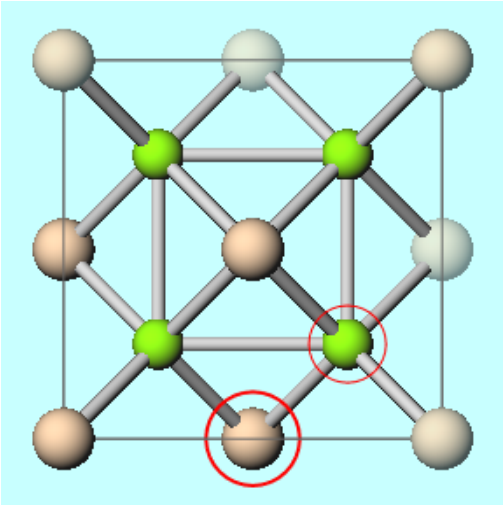
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

Please refer to QE Basic Tutorial for the basic operation method.

For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'.

A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.
B. Enter '`boltztrap_qe`' in **Project name** and click **Save**.
C. Click **File | Import | Sample File | mg2si.cif**.
    - If you wish to load a different file at this stage, use **File | Import File** instead.
D. In **Import File** dialog, click **Discard and import**.



B. Execution of Calculation

A. Select **Quantum ESPRESSO** from **Solver** in Toolbar and click  (**Workflow Setup**).

B. To reduce calculation time, click **Yes** when asked if you want to convert to a primitive cell. The converted structure will appear in Viewport. Click **OK** when 'Successfully converted lattice.' is displayed.

C. Set **# of bands** to “100% more”, select the **Pseudo file** as pbe-mt_fhi.upf, and set **Precision** to “High” (or “Medium” if you prefer faster calculations with lower precision). Then, check both **Metal** and **DOS**.

D. Click the **+** button next to **# of Jobs** once to add a second job.

E. For the 2nd job, change **Task** to “NSCF” and click **Details**.

F. Set **K_POINTS (Spacing)** to 0.05 (or 0.1 for lower-precision and faster calculations), change **occupations** to tetrahedra, and click **OK**.

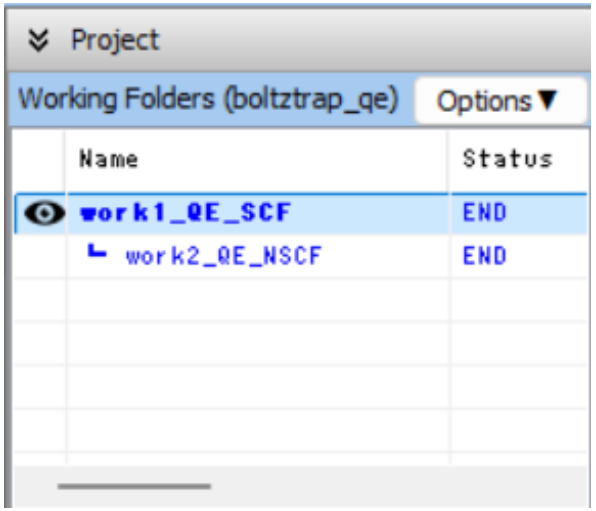
G. Click **OK** in **Quantum ESPRESSO Workflow Setup** window, then make appropriate settings in **Job Setting** window before clicking **Run**.

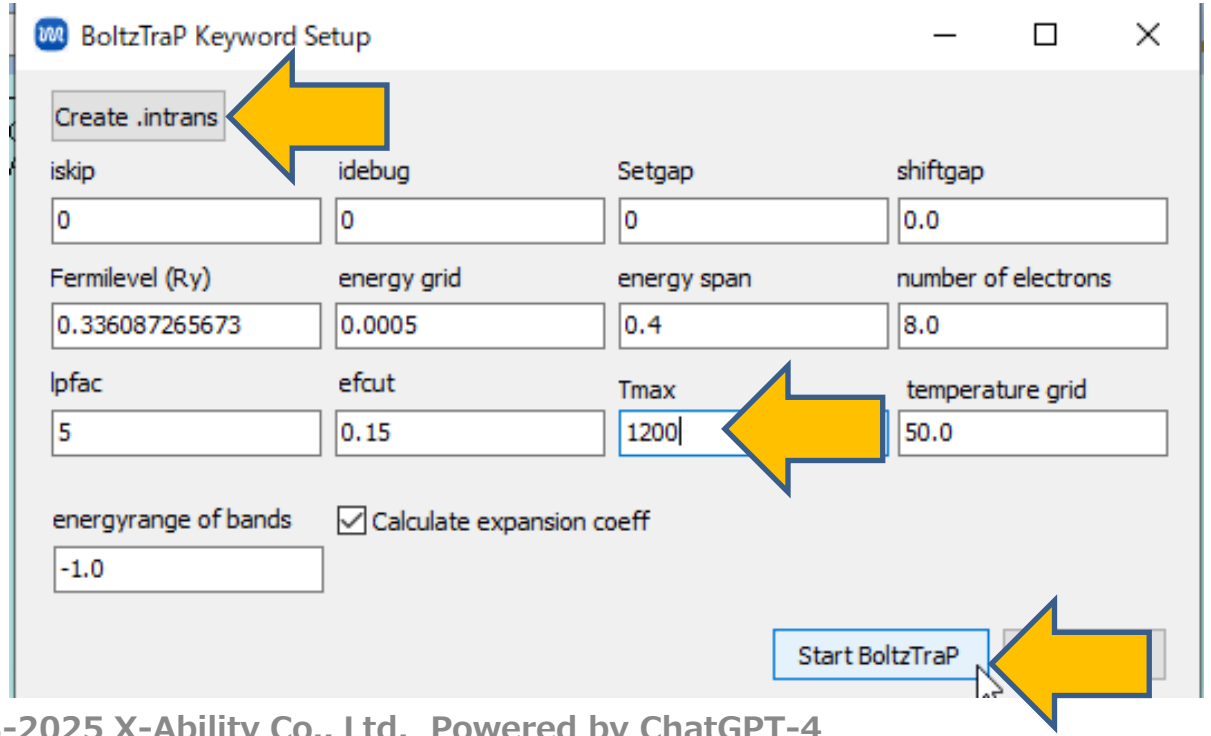
C. Result Analysis

A. After **the status** of **work2_QE_NSCF** in **Working Folders** changes to **END（blue）**, Click **Solid | Quantum ESPRESSO | BoltzTraP | Configure &Run…**

B. Click **Create .instrans**, then select and open pw.pwout from the work2_QE_NSCF folder.

C. Change **Tmax** to '1200', then click **Start BoltzTraP**. A console window will open, and the BoltzTraP process will run for a while.



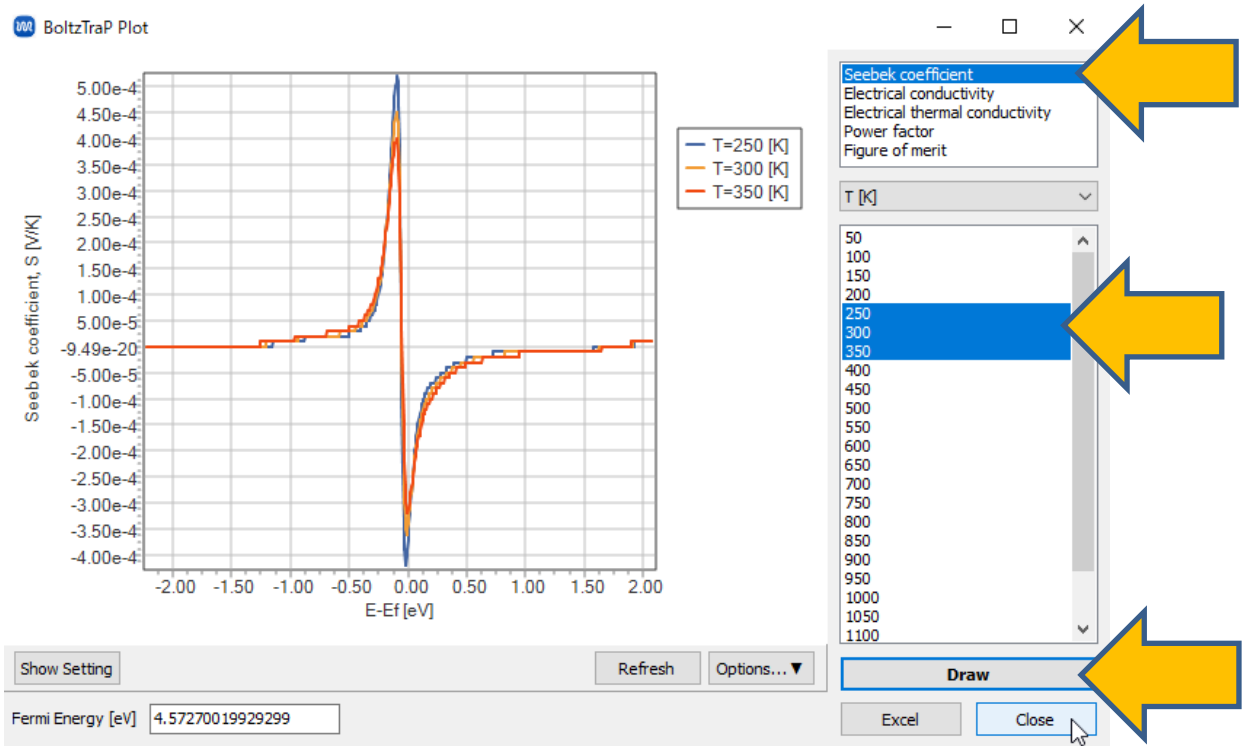


C. Result Analysis

A. After the BoltzTraP process finishes and the console window closes, click **Solid | Quantum ESPRESSO | BoltzTraP | Import Results…**. Then select the pw folder inside the work2_QE_NSCF directory and click **OK**.

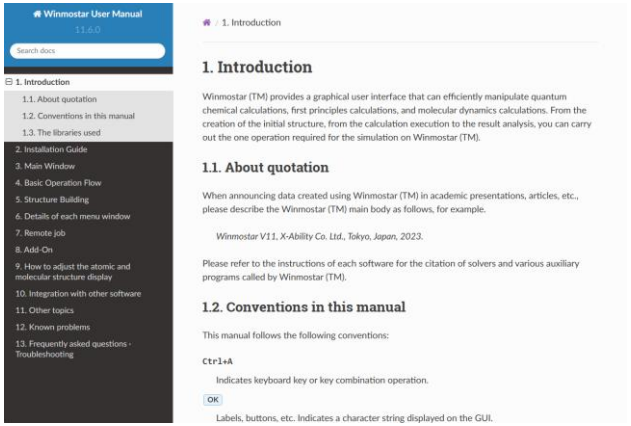
B. In the list at the top right, click **Seebeck Coefficient**. Then, in the list below it, hold Ctrl and click to select multiple temperatures: **250, 300,** and **350**.

C. Click **Draw** to show the graph.



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.