winmostar tutorial

Quantum ESPRESSO
Löwdin Charges/Bader Charges

V11.6.5

9 April 2024 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.
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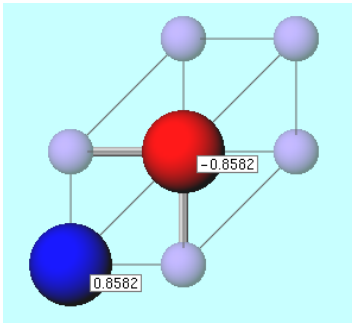
Overview

- This tutorial requires Winmostar V11 Professional Elite Edition for calculating Bader charges, while Löwdin charges can be calculated with the Economy and Premium editions as well.
- In this tutorial, we will perform an SCF calculation for a NaCl crystal and obtain the Löwdin and Bader charges derived from population analysis.



Note :

- The choice of k-points, number of bands, type of pseudopotential, and cutoff energy can impact the calculation results.
- There are various methods for population analysis in electronic state calculations, and Löwdin and Bader charges are calculated based on different design philosophies. Therefore, it is not a problem if the two do not match.

◆ For a detailed explanation of Quantum ESPRESSO's calculation methods and settings, please see the following article from our company: https://qiita.com/xa_member

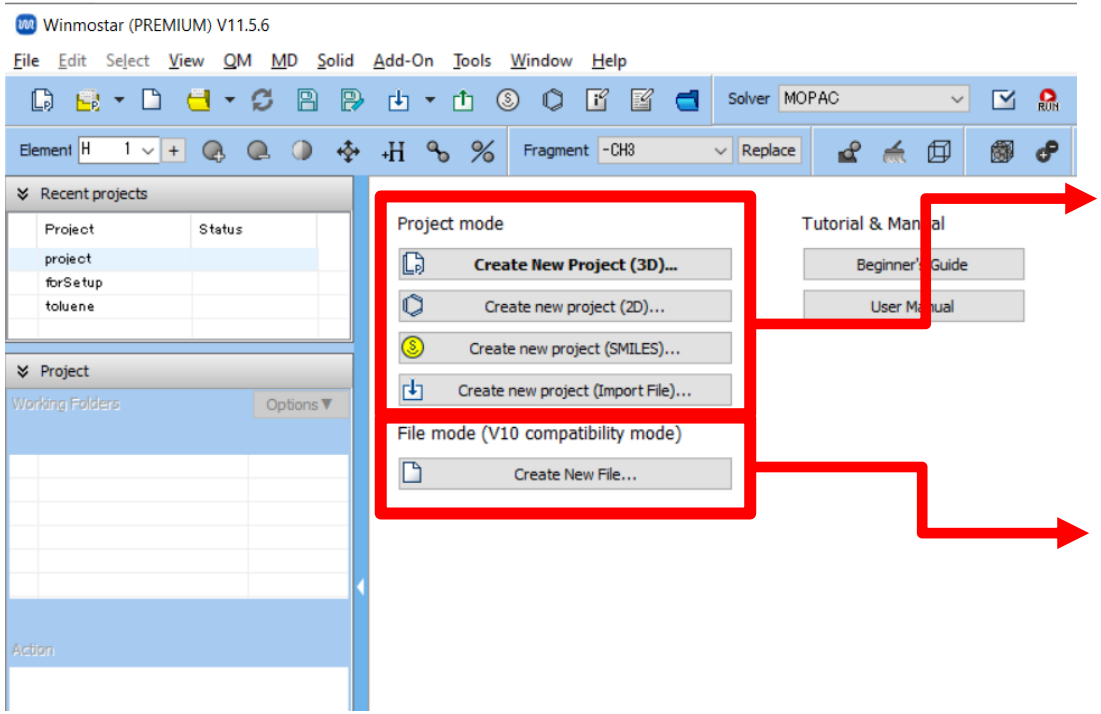
Preference of Operating Environment

- 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.

Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to [Quantum ESPRESSO tutorial for version 10].



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.

A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

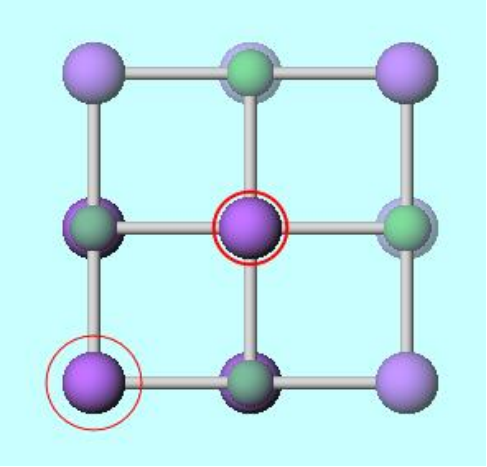
B. Enter '`qe_nacl_charge`' in **Project name** and click **Save**.

For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'.Here, we load an existing molecular structure file.

C. Click **File | Import | Sample File | nacl.cif**.

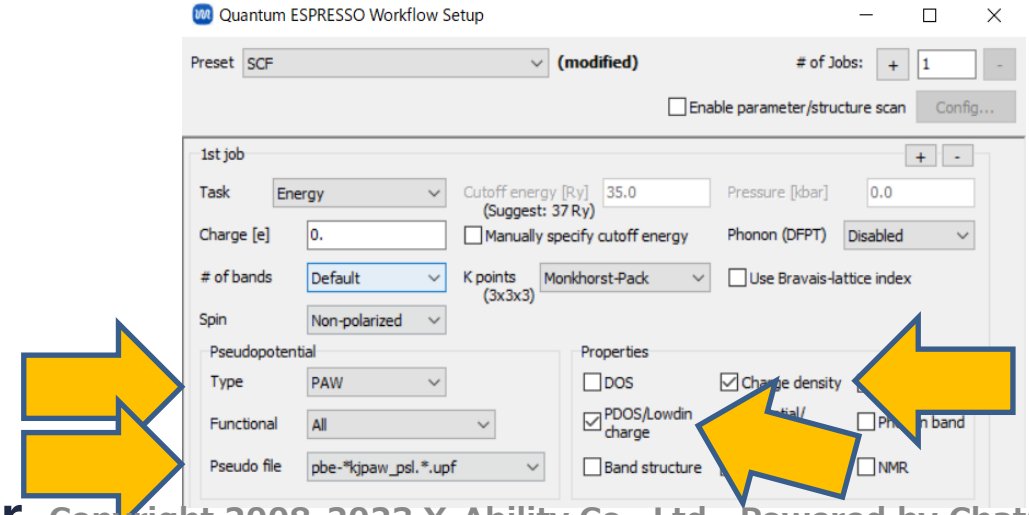
- If you wish to load a different file at this stage, use **File | Import File** instead.

D. In **Import File** dialog, click **Discard and import**.



B. Execution of Calculation

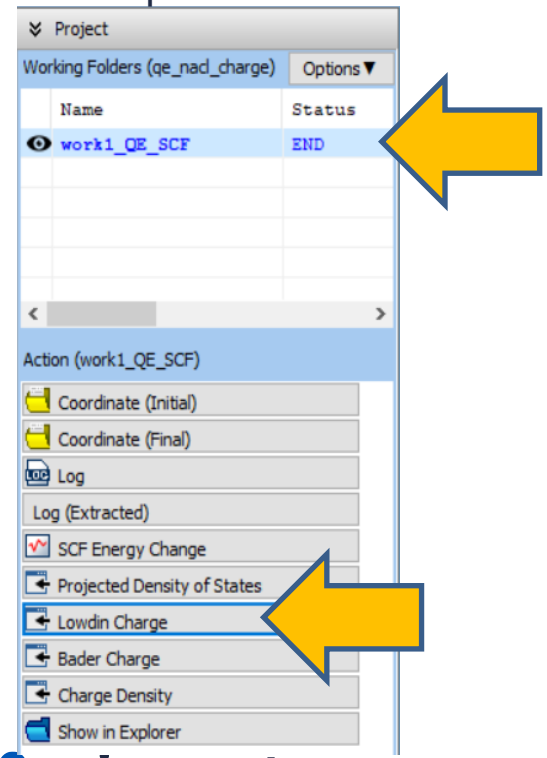
A. Select **Quantum ESPRESSO** from **Solver** and click **(Workflow Setup)**.
B. Click **Yes** when prompted with 'Current cell can be converted to primitive cell...Do you want to convert?'
C. Since Bader charge calculations are only compatible with PAW, change **Type** of **Pseudopotential** to **PAW** and change **Pseudo file** to **pbe-*kjpaw_psl.*.upf**.
   – If the PAW pseudopotential for the element you want to calculate does not appear, follow these steps to add the pseudopotential.
D. Check **PDOS/Lowdin charge** and **Charge density** under **Properties** (**Charge density** is required for calculating Bader charges).
E. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.

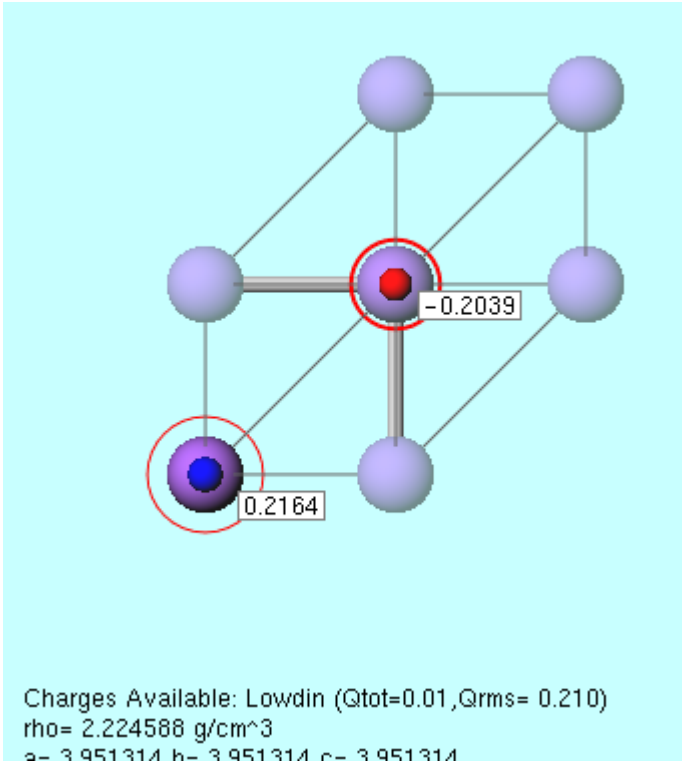


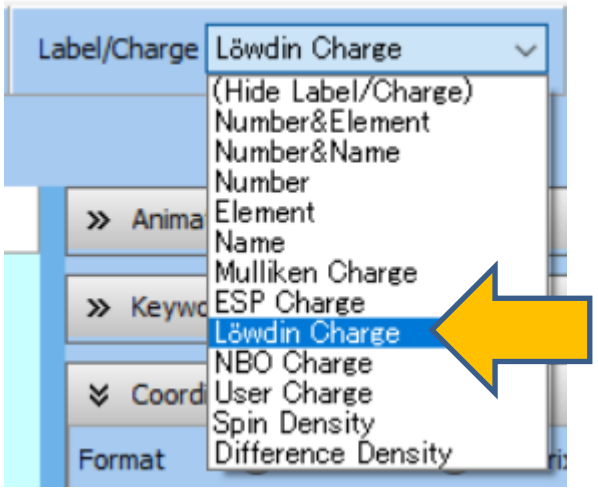
C. Result Analysis (Löwdin Charges)

A. Once **the status** of work1_QE_SCF folder changes to **END** or **END(-)**, click 'work1_QE_SCF' and select **Lowdin Charge** from **Action**.

B. The calculated Lowdin charges will be displayed in Viewport. If not displayed, change **Label/Charge** in the first row of Toolbar on the right to 'Lowdin Charge'. The total charge (**Qtot**) and the root mean square (**Qrms**) will be displayed at the bottom of Viewport.



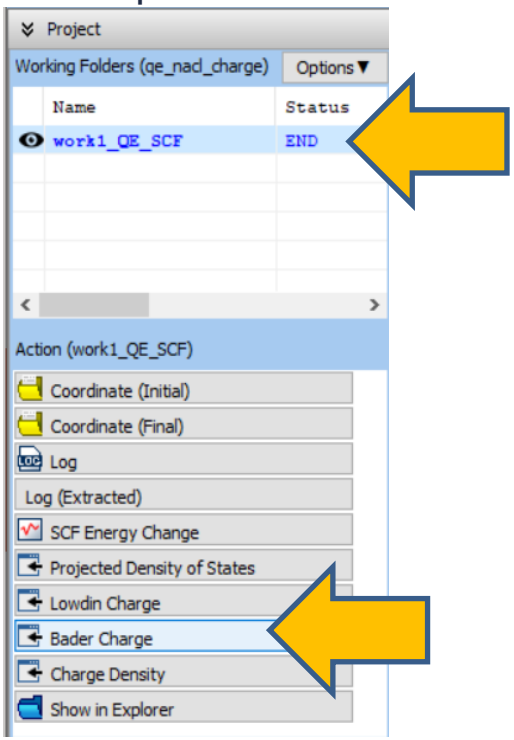


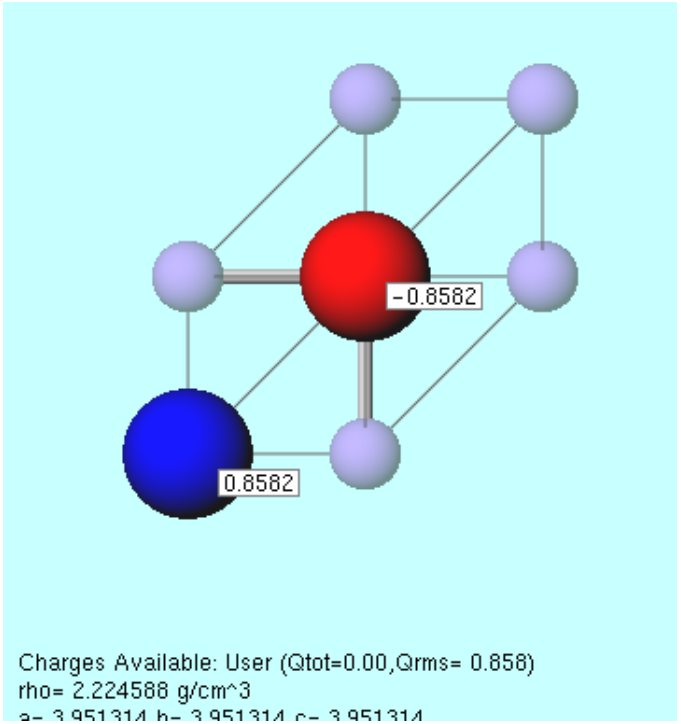


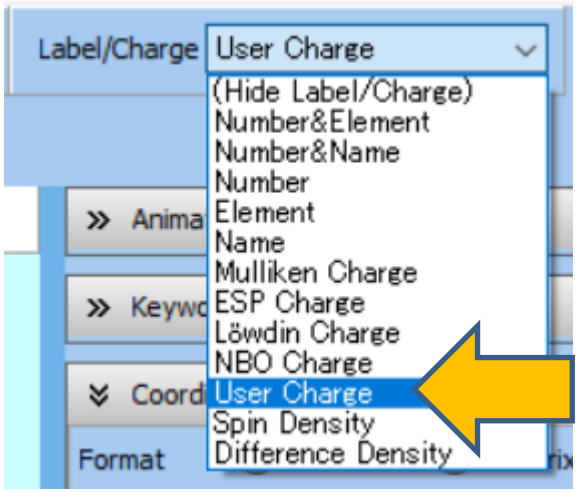
C. Result Analysis (Bader Charges)

A. Click **Bader Charge** in **Action**. (This is only possible with Winmostar V11 Professional Elite Edition)

B. The calculated Bader charges will be displayed in Viewport. If not displayed, change **Label/Charge** in the first row of Toolbar on the right to 'User Charge'. The total charge (**Qtot**) and the root mean square (**Qrms**) will be displayed at the bottom of Viewport.

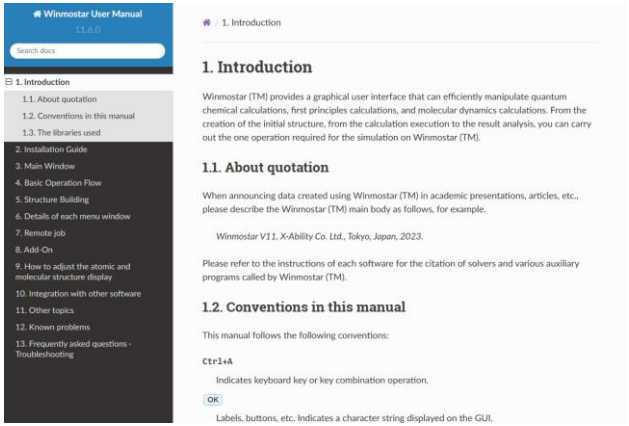






Finally

- 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.)
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