winmostar tutorial

FDMNES
XANES Spectra

V11.6.5

13 March 2024 X-Ability Co., Ltd.

About This Document

- 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.
- 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 from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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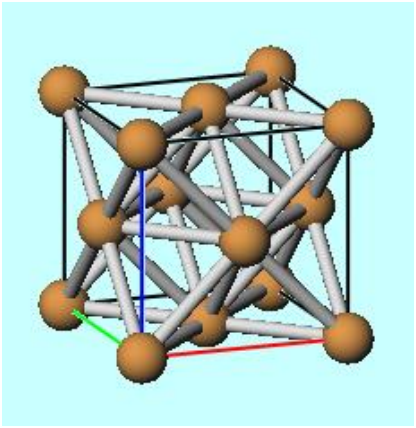
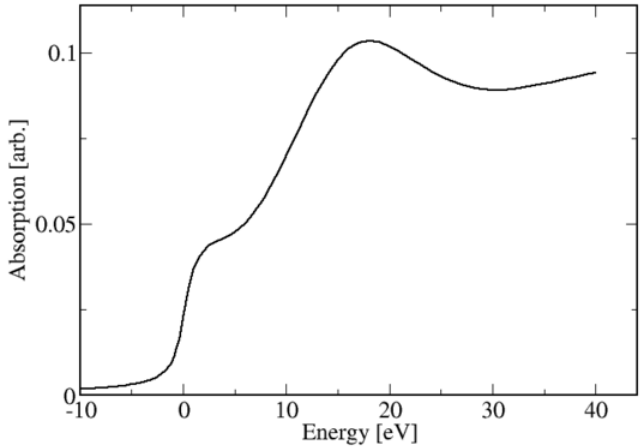
Overview

- In this tutorial, we use FDMNES, a freeware specialized in calculating X-ray spectra, to compute the XANES spectrum of a copper crystal.

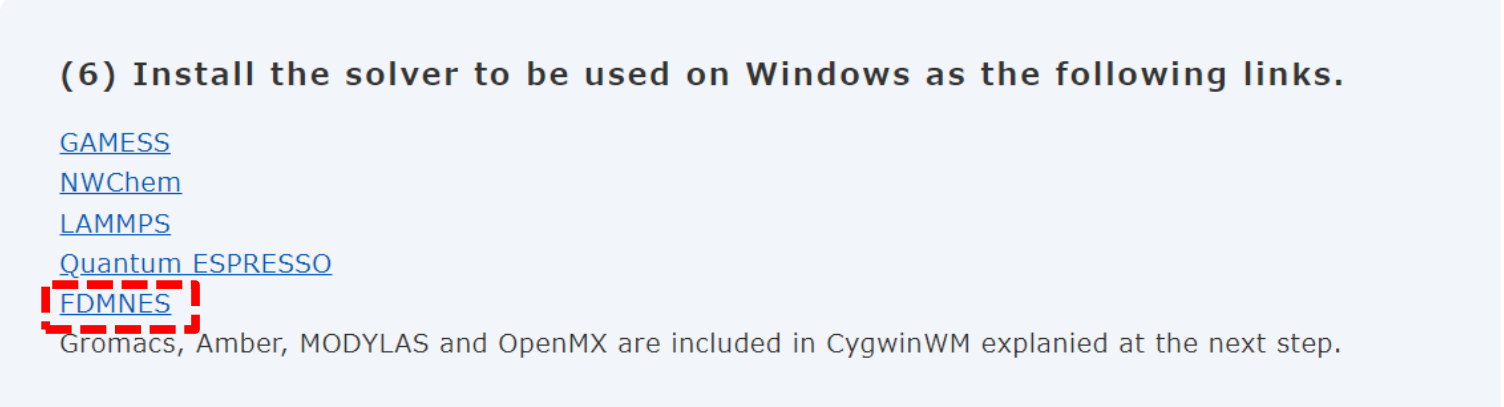




- Note:
- Structure optimization needs to be performed using other software such as Quantum ESPRESSO or OpenMX.
- The cluster radius and computational method can affect the calculation results.
- Caution is needed when comparing XANES spectra derived from simulations with different computational methods and basis sets for wave functions.

Preference of Operating Environment

- To use this feature, FDMNES setup is required.
- Follow the setup instructions for FDMNES for Windows at
  https://winmostar.com/en/installation/

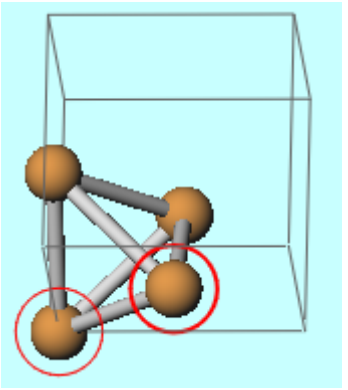


A. Setting Up & Running FDMNES

A. Click **File | Open File**.

B. Open **cu.cif** from the samples folder. (By default, it's located at **C:¥winmos11¥samples¥cu.cif**).

※ This CIF file can be created using the crystal builder.
Follow the operating instructions in the crystal modeling tutorial and create a unit cell based on the following information.



Regarding the Cu Unit Cell
Crystal system : Cubic
Space group : Fm-3m (225)
Lattice constants : a=3.6149 Å
Asymmetric unit : Cu (0.0 0.0 0.0)

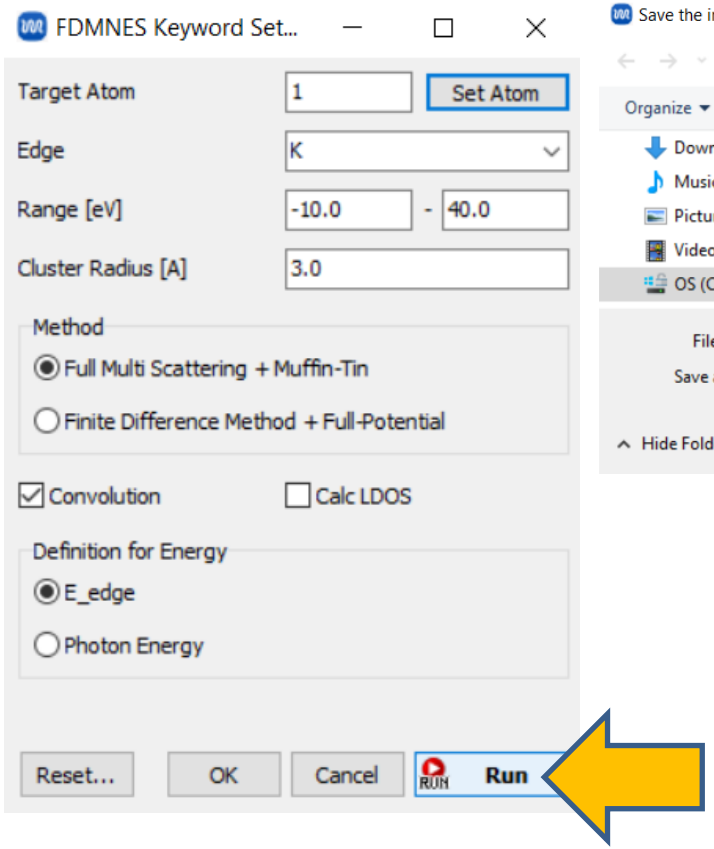
C. Select **FDMNES** from Toolbar's **Solver**.

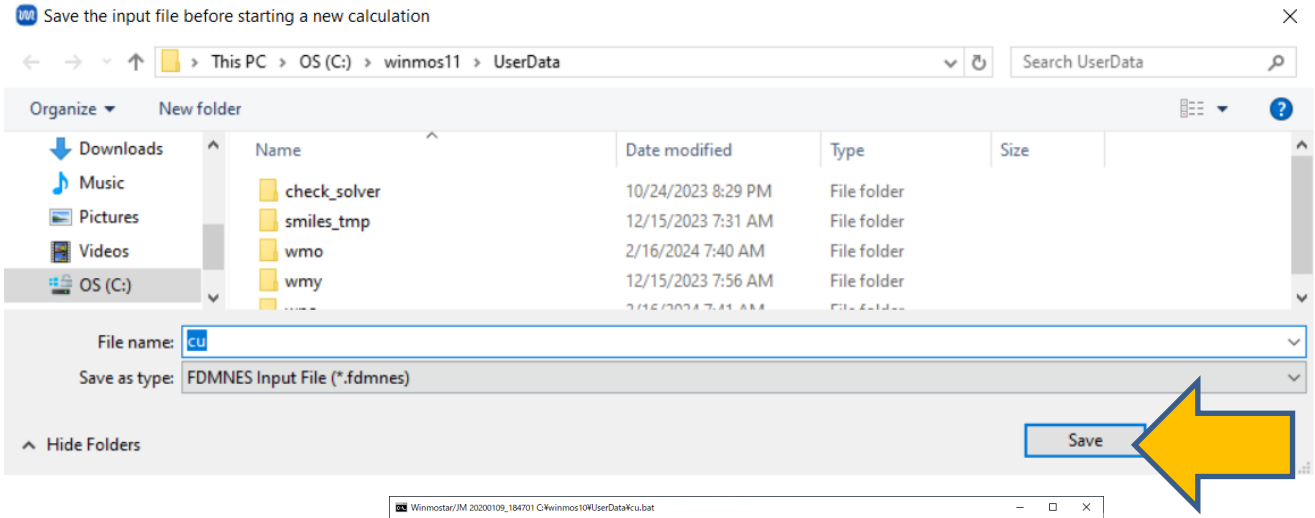
D. Click (**Keyword Setup**).

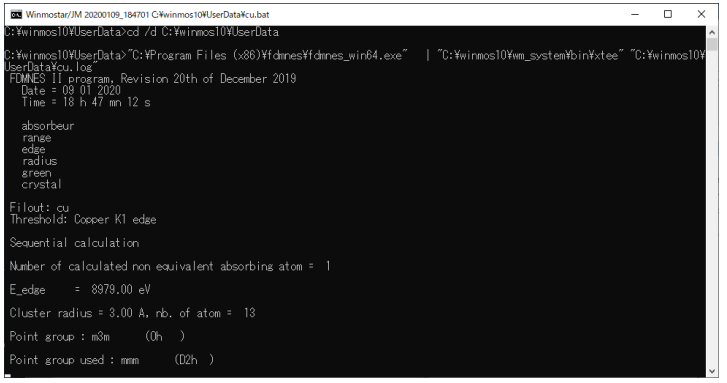
A. Setting Up & Running FDMNES

A. Click **Run** with the default settings.

B. When prompted for a file name and click **Save**, and then create the input file and start the calculation.





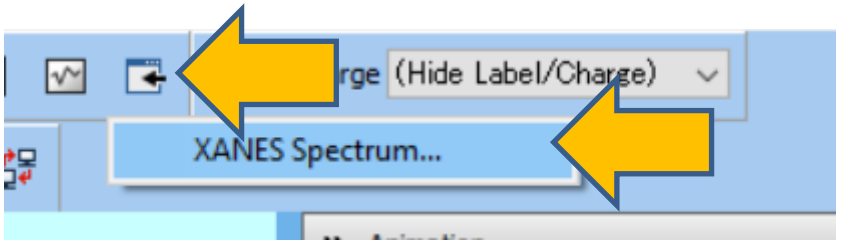


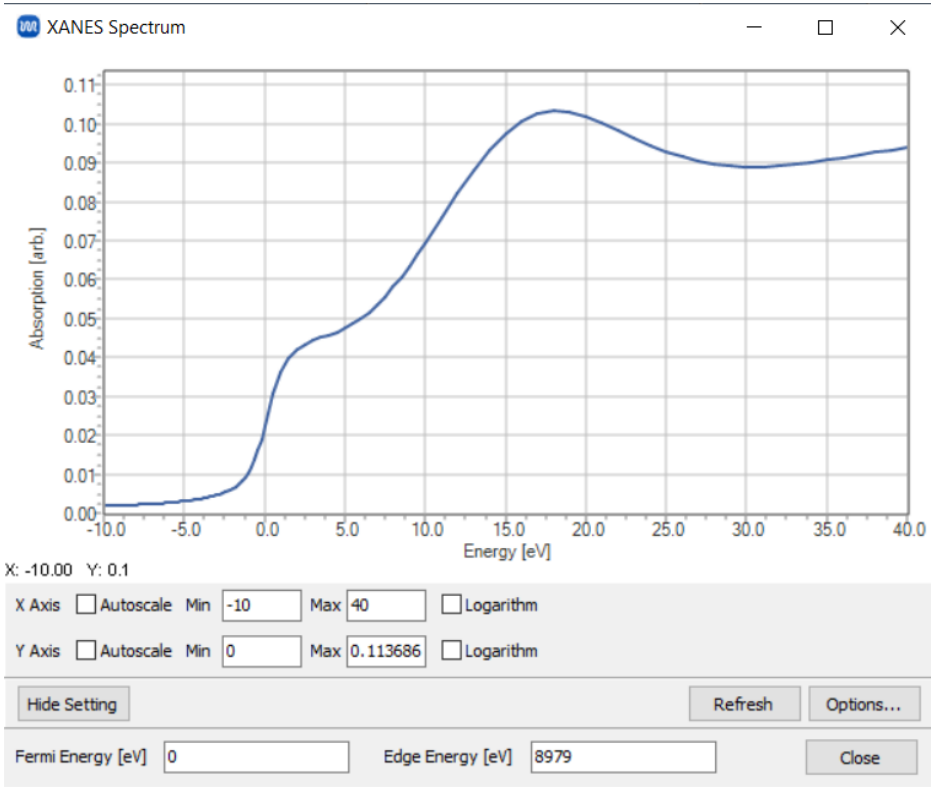
B. Displaying the XANES Spectrum

A. After the calculation is completed, click  (**Result Analysis**) **| XANES Spectrum**.

B. Select the default chosen file to obtain the calculated XANES spectrum (as shown on the right).

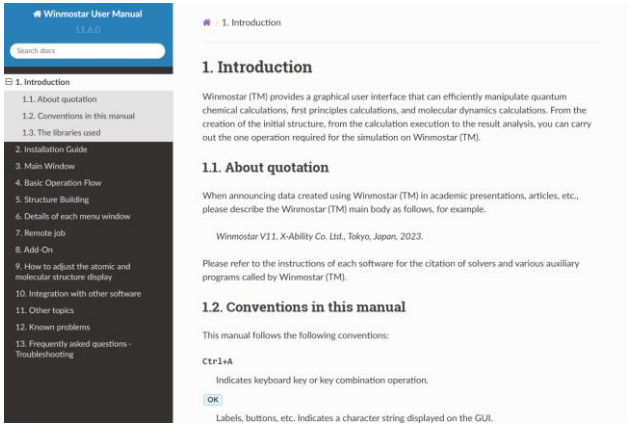
・ Be cautious if using versions of FDMNES prior to June 23, 2016, as the x-axis may not be shifted to the Fermi energy.





Troubleshooting and Additional Resources

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



Winmostar User Manual

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