

 winmostar tutorial

FDMNES XANES Spectra

V11.6.5

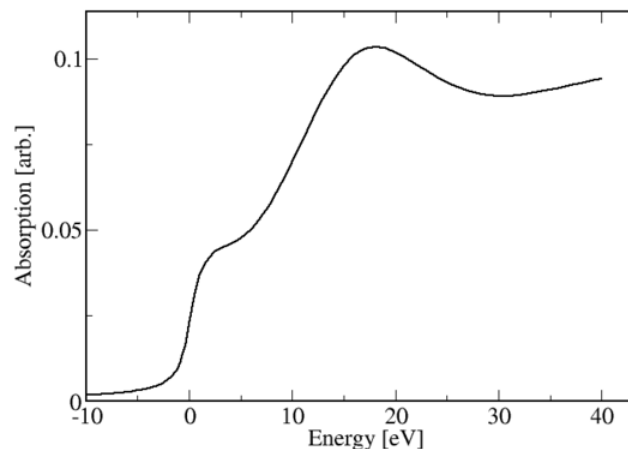
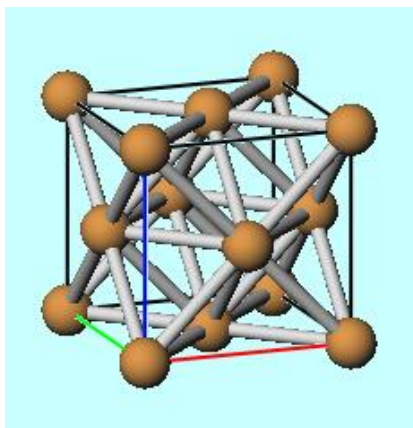
13 March 2024 X-Ability Co., Ltd.

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/>

(6) Install the solver to be used on Windows as the following links.

[GAMESS](#)

[NWChem](#)

[LAMMPS](#)

[Quantum ESPRESSO](#)

[FDMNES](#)

Gromacs, Amber, MODYLAS and OpenMX are included in CygwinWM explained at the next step.

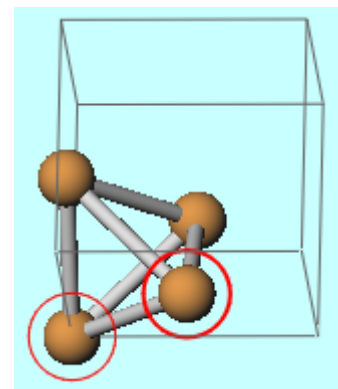
A. Setting Up & Running FDMNES

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

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

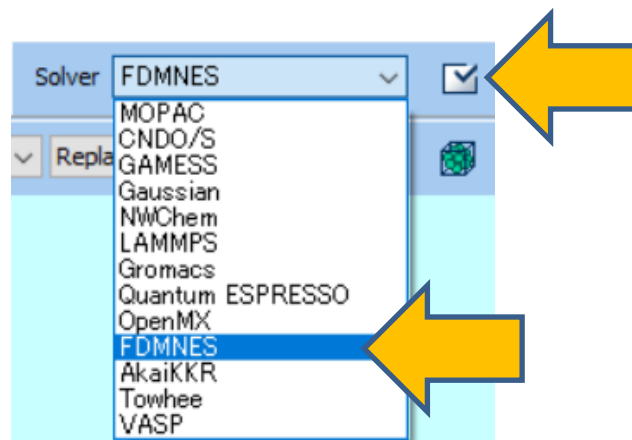
※ This CIF file can be created using the crystal builder. Follow the operating instructions in the crystal modeling tutorial and create a unit cell based on the following information.

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

- Click **Run** with the default settings.
- When prompted for a file name and click **Save**, and then create the input file and start the calculation.

The image shows the FDMNES Keyword Set dialog box on the left and a Windows Explorer window on the right. The dialog box has the following settings:

- Target Atom: 1 (Set Atom button)
- Edge: K
- Range [eV]: -10.0 - 40.0
- Cluster Radius [Å]: 3.0
- Method: Full Multi Scattering + Muffin-Tin, Finite Difference Method + Full-Potential
- Convolution, Calc LDOS
- Definition for Energy: E_edge, Photon Energy
- Buttons: Reset..., OK, Cancel, **Run** (highlighted with a yellow arrow)


The Windows Explorer window shows the path: This PC > OS (C:) > winos11 > UserData. It displays a list of folders: check_solver, smiles_tmp, wmo, wmy. The File name field contains 'cu' and the Save as type is 'FDMNES Input File (*.fdmnes)'. A yellow arrow points to the Save button.

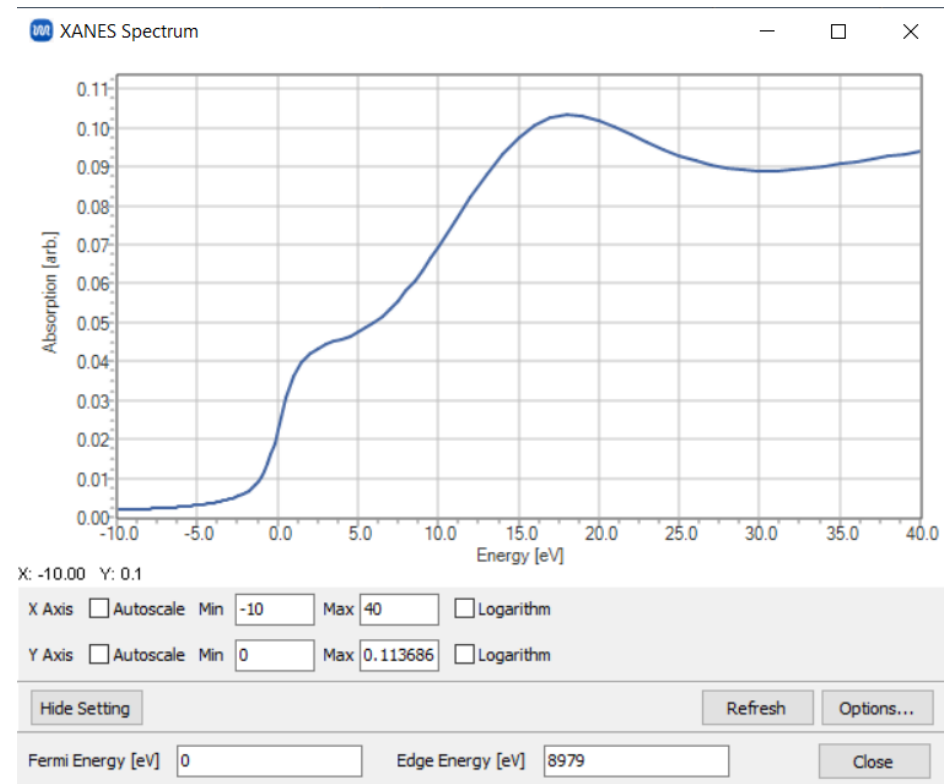
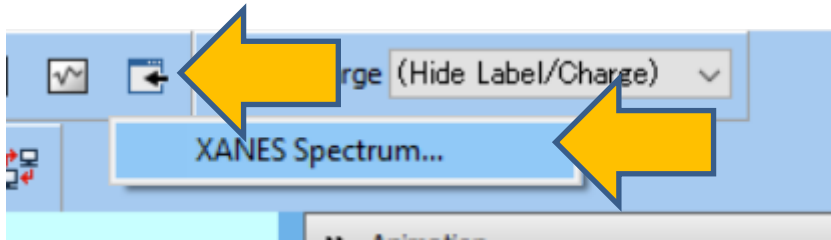
```
Winmostar/JM 2020109_184701 C:\winos10\UserData\cu.bat
C:\winos10\UserData>cd /d C:\winos10\UserData
C:\winos10\UserData>C:\Program Files (x86)\Yfdines\fdines_win64.exe | "C:\winos10\ym_system\bin\ytee" "C:\winos10\UserData\cu.log"
FDMNES 11 program, Revision 20th of December 2019
Date = 09 01 2020
Time = 18 h 47 mn 12 s

absorbeur
rise
edge
radius
areen
crystal

Fileout: cu
Threshold: Copper K1 edge
Sequential calculation
Number of calculated non equivalent absorbing atom = 1
E_edge = 8979.00 eV
Cluster radius = 3.00 Å, nb. of atom = 13
Point group : m3m (Oh )
Point group used : mm (O2h )
```

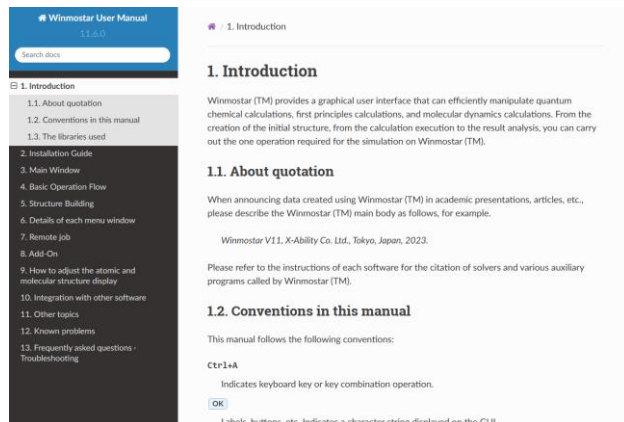
B. Displaying the XANES Spectrum

- 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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