

Winmostar tutorial  
FDMNES  
Cu crystal  
V8.007

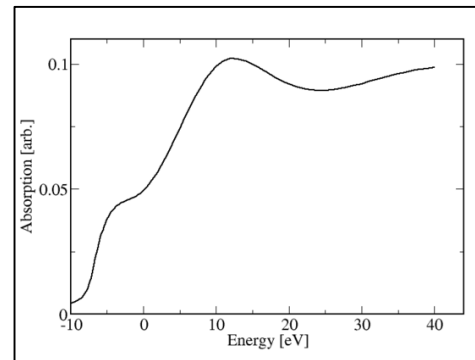
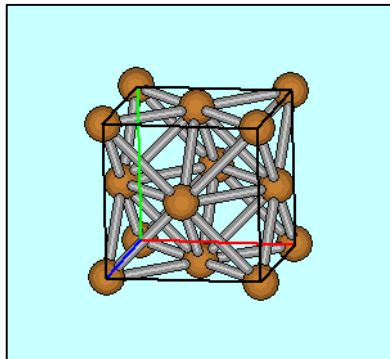
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# Summary

- This tutorial will show how to calculate the XAFS spectrum of a Cu crystal using the freeware FDMNES.



## Note:

- Structural optimization must be done with other software such as Quantum ESPRESSO, OpenMX.
- The cluster radius and calculation methods may affect calculation results.
- Precautions are necessary when comparing XAFS spectra calculated from simulations with varying calculation methods and/or wave function basis.

# I. Configure and execute FDMNES

1. Click **File | Open**.

2. Open **cu.cif** in samples folder. (e.g. C:\winmos8\samples\cu.cif)

You can also make the same CIF file using Crystal Builder.

See crystal modeling tutorial and use the following information.

Cu crystal

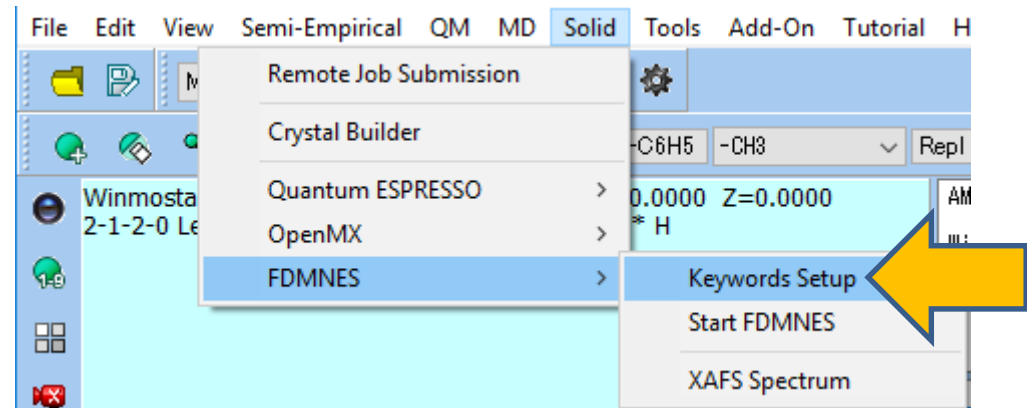
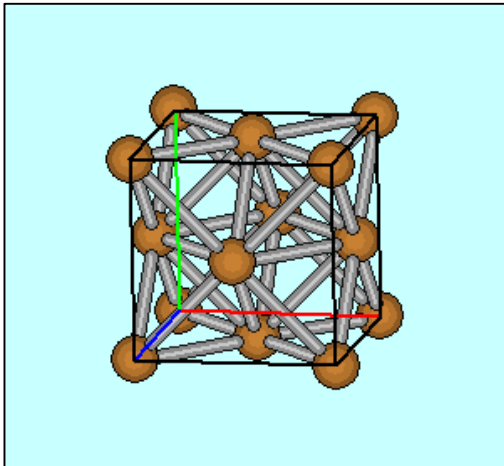
Crystal system : Cubic

Space group : Fm-3m (225)

Lattice constants : a=3.6149 Å

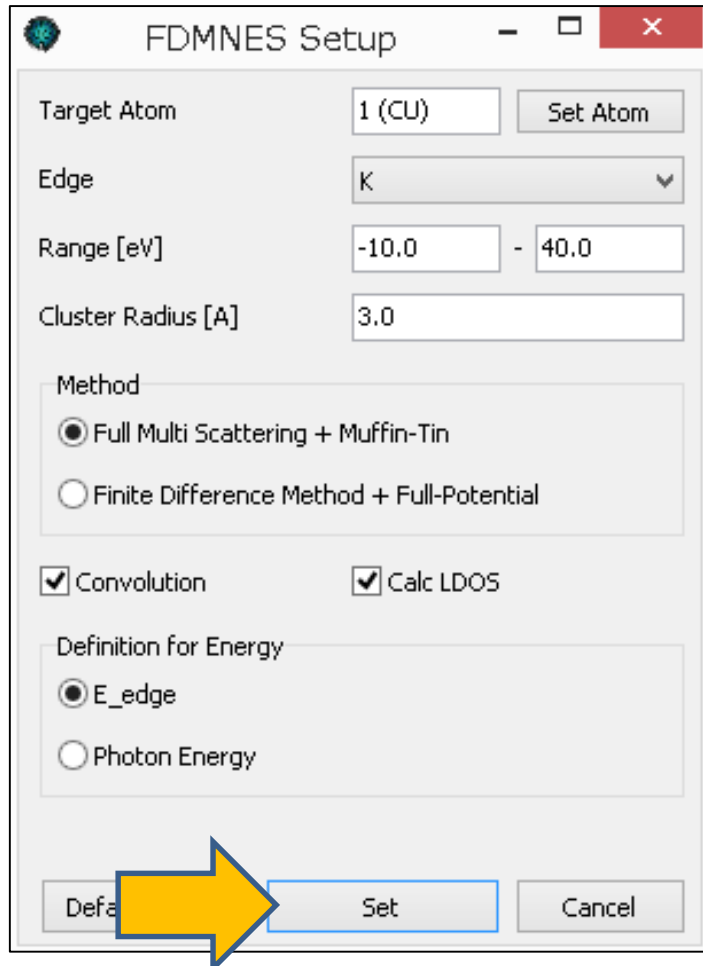
Asymmetric unit : Cu (0.0 0.0 0.0)

3. Click **Solid | FDMNES | Keywords Setup**.

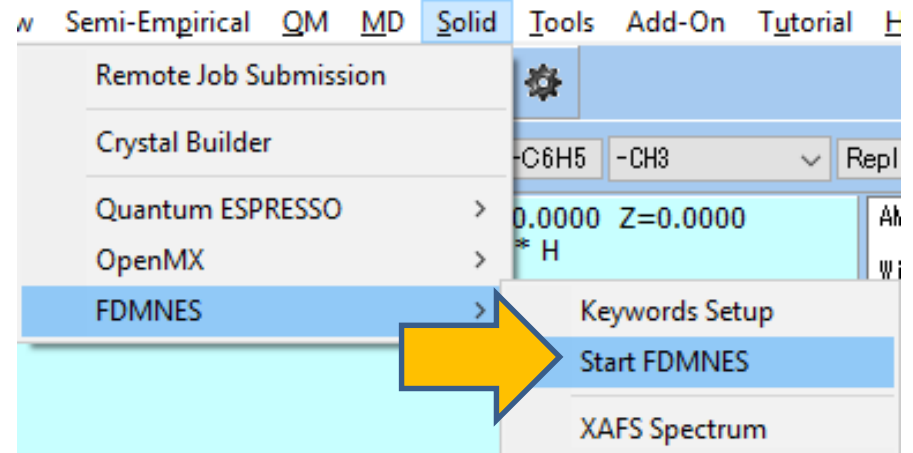


# I. Configure and execute FDMNES

1. Click **Set** with the default settings.



2. Click **Solid | Start FDMNES**.



## II. Visualize the XAFS spectrum

1. Click **Solid | XAFS spectrum**.
2. Select the output file suggested by default.  
The predicted XAFS spectrum will appear.

