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Winmostar tutorial

FDMNES

Cu crystal

V7.000

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Contents

I. Configure and execute FDMNES
II. Visualize the XAFS spectrum

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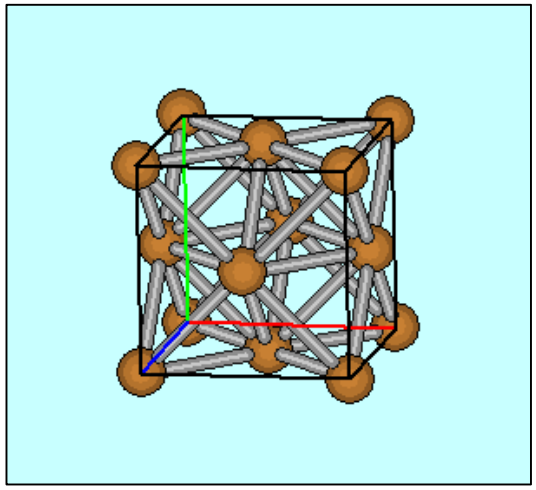
I. Configure and execute FDMNES

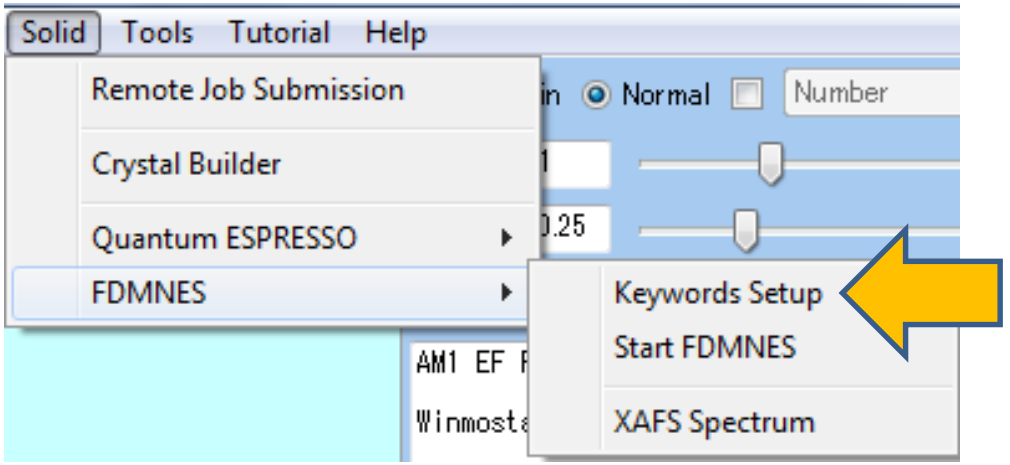
1. Click **File | Open**.
2. Open **cu.cif** in samples folder.（e.g. C:¥winmos7¥samples¥cu.cif）

   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**.





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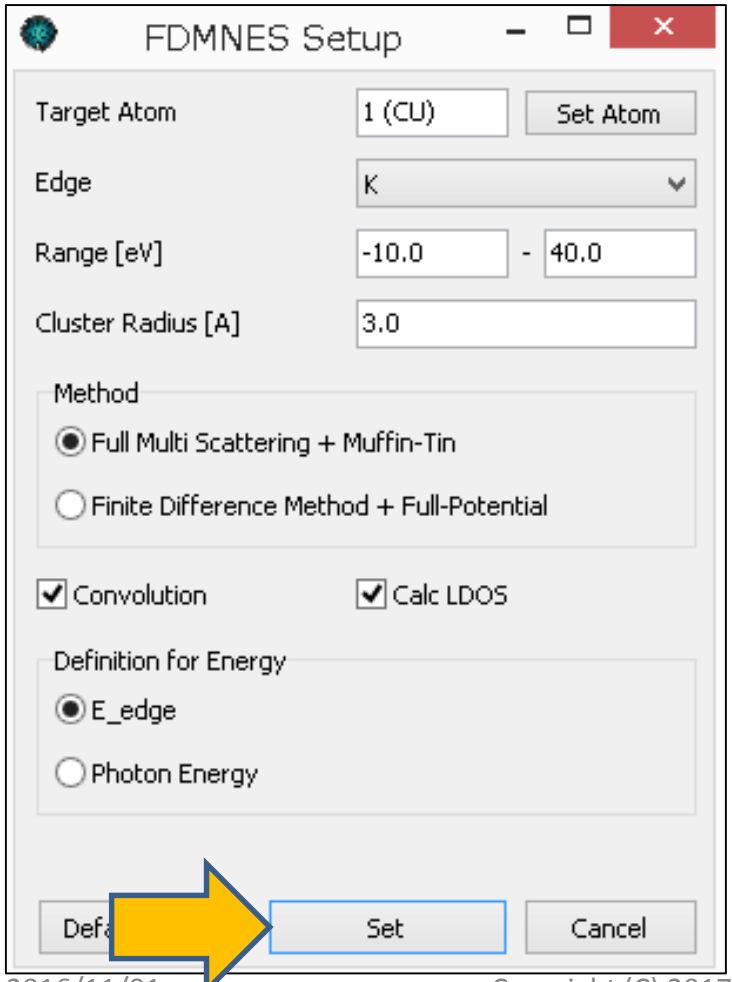
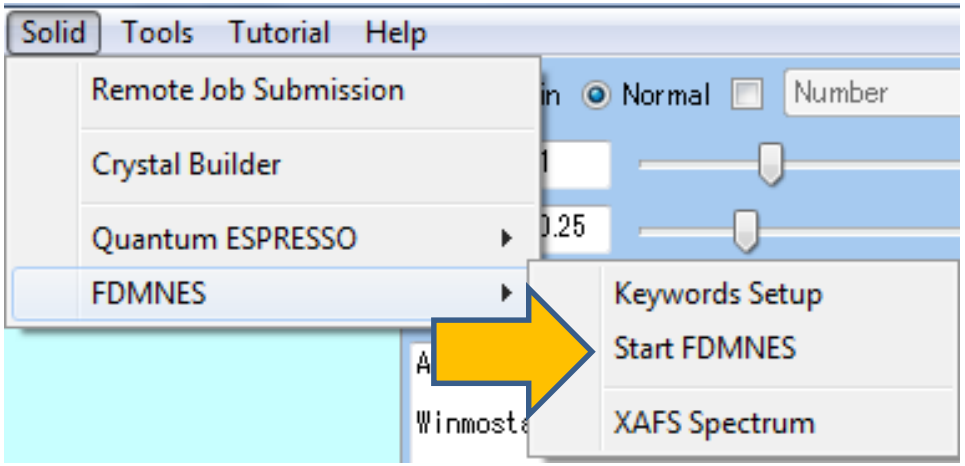
I. Configure and execute FDMNES

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



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



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II. Visualize the XAFS spectrum

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