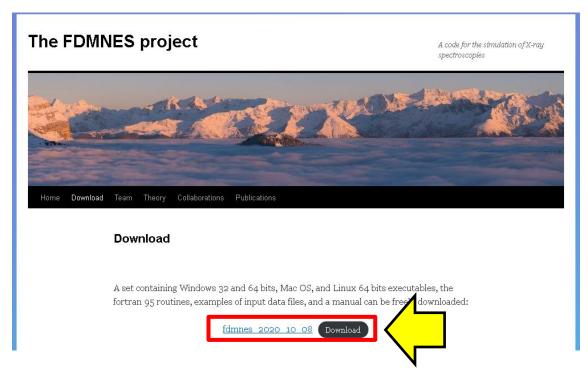
FDMNES for Windows Installation Manual

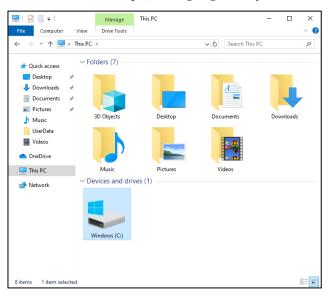
October 10, 2020

1. Installation of FDMNES

i. Go to the following site and download the zip file of the FDMNES package. http://fdmnes.neel.cnrs.fr/download/



ii. Unzip the downloaded zip file and move the generated "fdmnes" folder to an appropriate location. (In this example, we're going directly under the C:\.)



iii. To set the path for Winmostar to call FDMNES, click [Tools] \rightarrow [Preferences] in the Winmostar menu to open the Preferences panel.

Open the Preferences Panel [Program Path] tab, and click the [...] button under [FDMNES]. button of [FDMNES]. Register "fdmnes_win64.exe" in the fdmnes folder, and click [OK].

M Preference				- 0	×
Basic Edit	Calculation View Program Path				
Editor:	notepad		GAMESS(1):	C:¥Users¥Public¥gamess-64¥games	
Jmol:	C:¥jmol-11.5¥jmol.bat		GAMESS(2):	C:¥ff820_windows¥Firefly820.exe	
Mercury:	C:¥Program Files¥CCDC¥Mercury 1.		Gaussian:	C:¥g03w¥g03.exe	
POV-Ray:	C:¥Program Files¥POV-Ray¥v3.7¥bi		NWChem:	C:¥nwchem¥bin¥nwchem.exe	
OpenSCAD:	C:¥Program Files¥OpenSCAD¥open:		Cygwin:	C:¥cygwin_wm	
VMD:	C:¥Program Files (x86)¥University c		LAMMPS:	C:¥Program Files¥LAMMPS 64-bit 20	
MOPAC(1):	C:¥winmos10¥wm_system¥bin¥mop		MPICH2:	C:¥Program Files¥MPICH2¥bin¥mpie	
MOPAC(2):	C:¥winmos10¥wm_system¥bin¥mop		Quantum ESPRESSO:	C:¥Program Files¥Quantum ESPRES	
MOPAC(3):	C:¥winmos10¥wm_system¥bin¥mop		FDMNES:	C:¥fdmnes¥fdmnes_win64.exe	
MOSF:	C:¥winmos10¥wm_system¥bin¥mos		CONFLEX:	:ONFLEX¥bin¥flex7b3_win_x64.exe	
Restore All Settings Import Export OK Cancel Apply					

* By default, "C:\fdmnes\fdmnes_win64.exe" is displayed, but when using the 32-bit version, change it to "C:\fdmnes\fdmnes_win32.exe".

iv.

In some environments, a system error message may be displayed when executing FDMNES and it may not be possible to execute.

In that case, Get the Microsoft Visual C++ 2010 SP1 Redistributable Package (x64) from https://www.microsoft.com/en-US/download/details.aspx?id=13523

For 32 bits, Get the Microsoft Visual C++ 2010 SP1 Redistributable Package (x86) from https://www.microsoft.com/en-US/download/details.aspx?id=8328 As of April 22, 2020, if you visit the above link, Select English and click "Download", vcredist_x86.exe will be downloaded.

Double-click vcredist_x64.exe and follow the instructions to install it.

2. Installation of cygwin_wm

Download the cygwin installer and set up according to the contents of the link below. (Not necessary if cygwin_wm has already been set up.) <u>https://winmostar.com/en/gmx4wm_en.html</u>