LAMMPS for Windows Installation Manual

April 22, 2020

1. Get LAMMPS

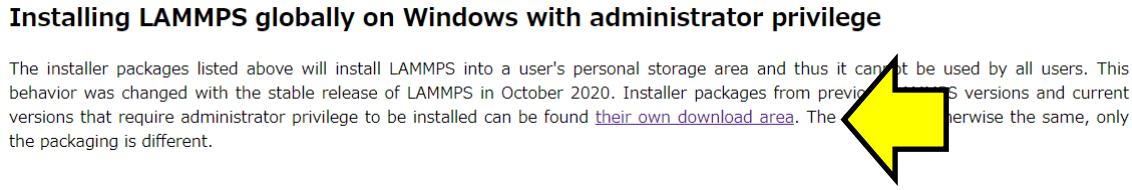
   i. Go to https://packages.lammps.org/windows.html. In rare cases, the connection may not work due to server maintenance, etc., but it will be restored in a few days to a week.

      ※ If it does not recover, download the installer from the following link.

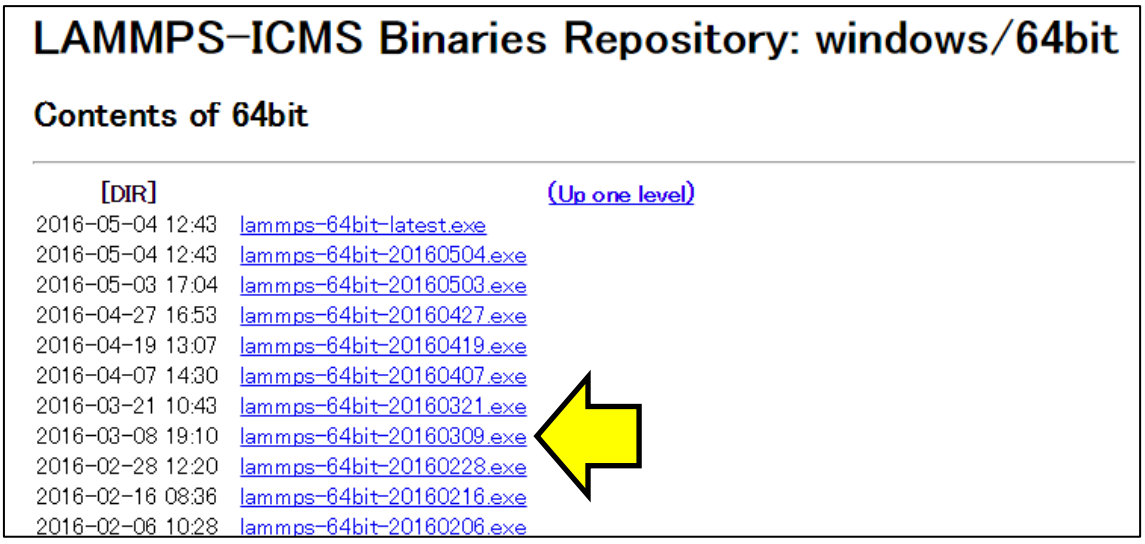
      https://winmostar.com/wm/cygwin_wm/packages/lammps-32bit-20160309.exe

      https://winmostar.com/wm/cygwin_wm/packages/lammps-64bit-20160309.exe

   Scroll down to **Installing LAMMPS globally on Windows with administrator privilege** and click on [their own download area].



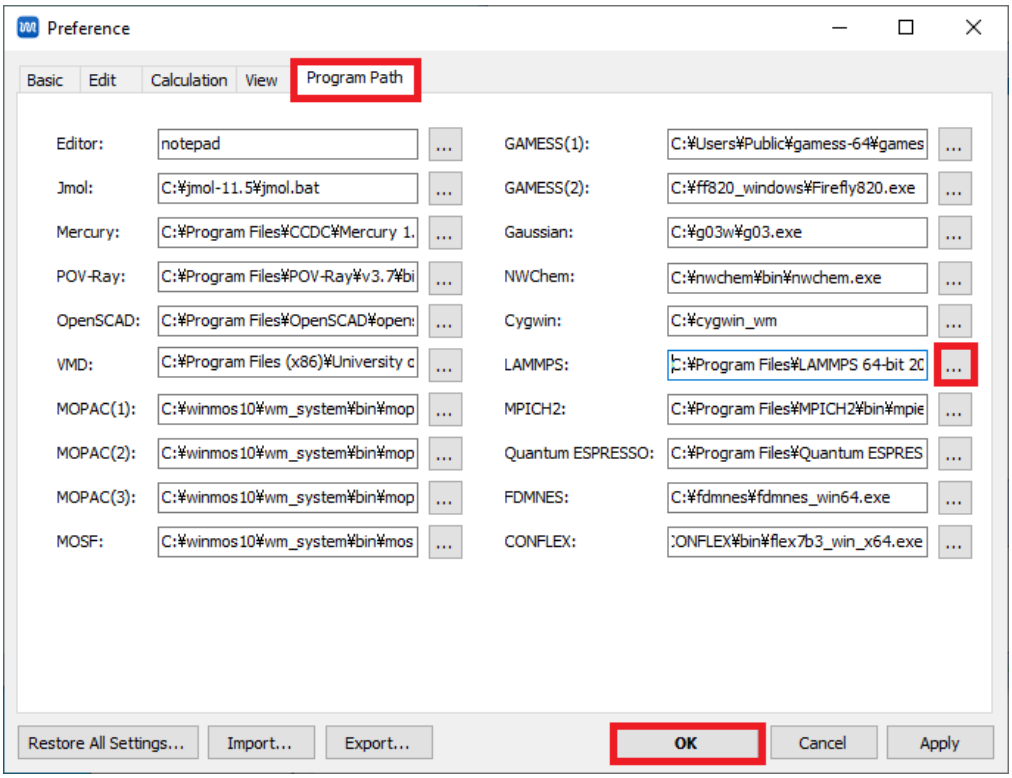
   ii. Click directory link of [64bit] or [32bit] and save lammps-64bit-20160309.exe for 64bit or lammps-32bit-20160309.exe for 32bit.



   iii. Double-click the saved exe file and follow the instructions.

   iv. To set the path for Winmostar to call LAMMPS, click [Tools] → [Preferences] in Winmostar to open the Preference panel. Open the [Program Path] tab of the Preference Panel, and click the [...] button of [LAMMPS] to register the LAMMPS executable file (lmp_serial.exe). Register the LAMMPS executable

file (lmp_serial.exe), and click [OK].



※By default, it is displayed as

C:\Program Files\LAMMPS 64-bit 20160309\bin\lmp_serial.exe. If you want to use 32bit one, change it to C:\Program Files\LAMMPS 32-bit 20160309\bin\lmp_serial.exe, etc.

2. Obtain and set up cygwin_wm (not necessary if cygwin_wm has already been set up)

   Download the cygwin_wm installer from the following link and set up.

   https://winmostar.com/en/gmx4wm_en.html

3. Obtain and install MPICH (required only if you want to run LAMMPS in parallel)

   i. Click [mpich2-1.4.1p1-win-ia32.msi] or [mpich2-1.4.1p1-win-x86-64.msi] to download the MSI file (if the extension is changed, revert to .msi), depending on the OS. If LAMMPS is 32-bit, select 32-bit MPICH (if it is 64-bit, select 64-bit).

   ii. Double-click on the saved MSI file and follow the instructions. If the installation fails, download .NET Framework 3.5 from https://www.microsoft.com/en-US/download/details.aspx?id=21. Windows 8.1/10 comes with .NET Framework 4.5 by default, but you need to install 3.5 separately.

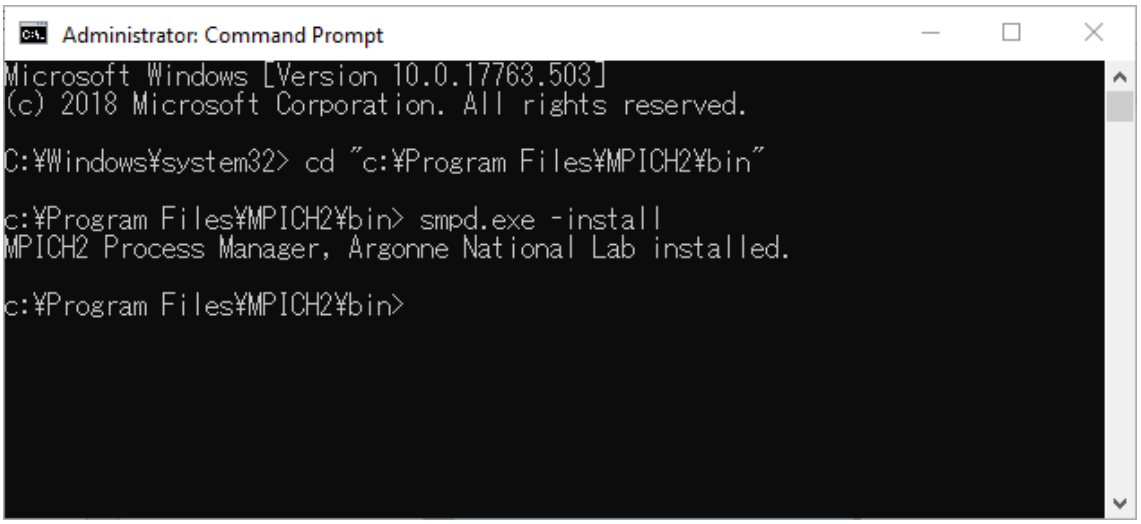
   iii. Start a command prompt from the start menu with administrative privileges.

   iv. Go to the folder where you installed MPICH.

   C:\> cd “C:\Program Files\MPICH2\bin”

   v. Execute the MPICH setup command (smpd.exe).

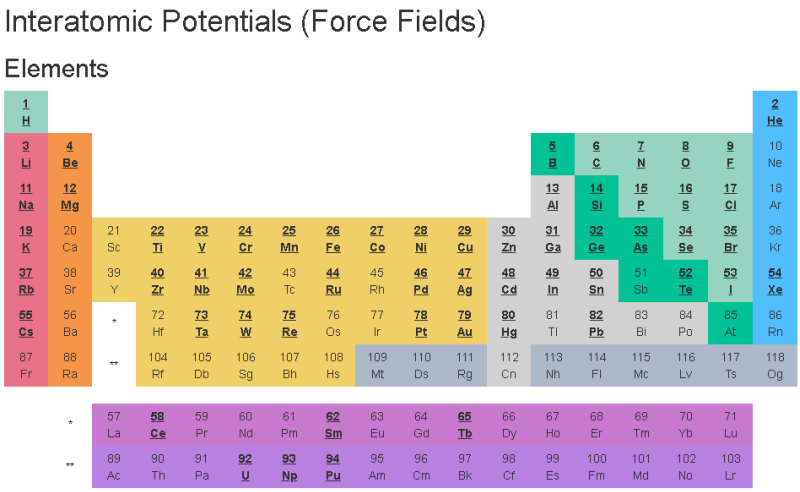
C:\Program Files\MPICH2\bin> smpd.exe -install



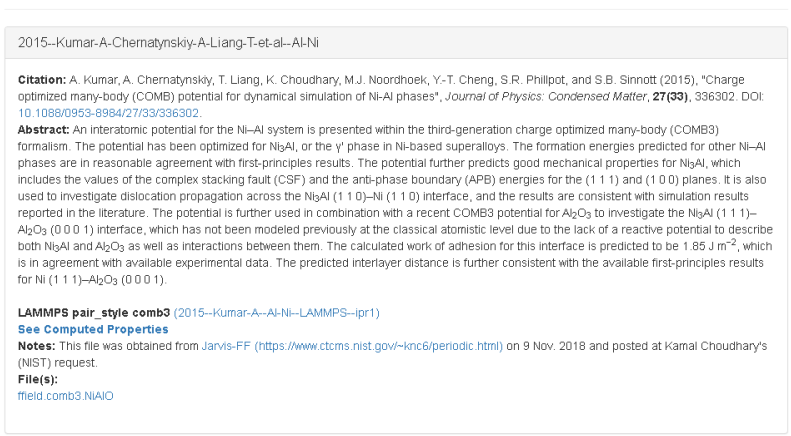
vi. (6) Click [Tools] → [Preferences] in Winmostar to open the Preference panel. Open the [Program Path] tab in the Preference Panel, and click the [...] button for [MPICH2]. Register the MPICH executable file (mpiexec.exe) and click [OK].

4. Obtain and install potential files for inorganic compounds (if necessary)

   i. Go to the website [NIST Interatomic Potentials Repository](), and click an element of you want to calculate.



   ii. Search the term including all elements you want to calculate.

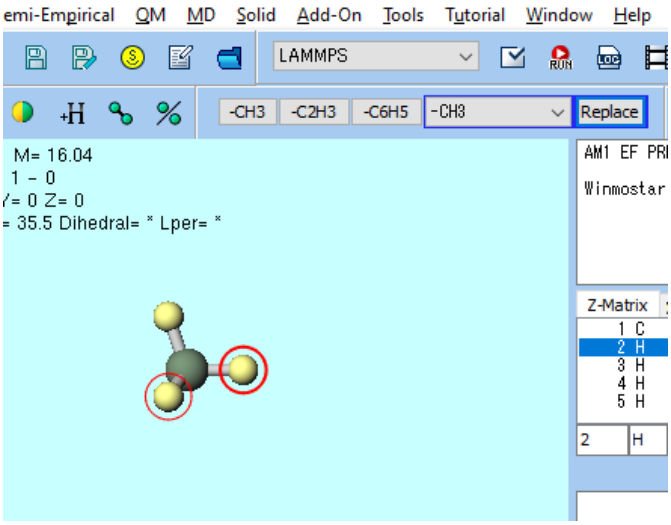


   iii. Right-click the link of "Files(s):", and save the file.

   iv. Copy the downloaded file to the Potentials folder in your LAMMPS installation folder (default: C:\Program Files\LAMMPS 64-bit 20160309\Potentials).

5. Simple operation check

i. Click [File]-[New] in the main menu of Winmostar, and then click [Replace] button at the upper center of the main window to create a methane molecule.



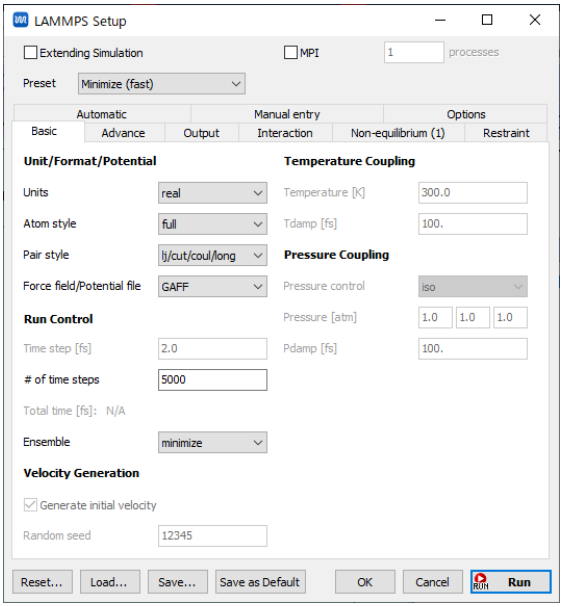
ii. Click on [MD]-[LAMMPS]-[Configure] and you'll see "Some molecules do not have charges. Do you want to assign charges now?" In the dialog box, press [Yes] button.

iii. A dialog box with "Assign charges" will appear. Press [OK] with the default value.

iv. A dialog box with "Create Cell" will appear. Press [OK] with the default value.

v. A dialog box with "Assign force field parameters" will appear. Press [OK] button with the default value.

vi. Click the [Run] button at the bottom right of the LAMMPS Setup window.



vii. A save dialog opens, and when you save it with a suitable name, a black terminal window opens and a lot of messages flow. After a while, the process is over and the terminal window closes.

viii. Click [MD]-[LAMMPS]-[Open Log File (log)] and open the file selected by default in the dialog. When the LAMMPS calculation succeeded, you will see the statistics of the calculation at the end of the opened text file.