

# OpenMX Viewer: what you can do

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# Manual of the OpenMX Viewer

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The OpenMX Viewer (Open source package for Material eXplorer Viewer) is a web-based graphical user interface (GUI) program for visualization and analysis of crystalline and molecular structures and 3D grid data in the Gaussian cube format such as electron density and molecular orbitals.

<http://www.openmx-square.org/viewer/>

The document provides the usage of the OpenMX Viewer.

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Feb. 27, 2026

# On license and citation of the related paper

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- The OpenMX Viewer has been released under the practice of the GNU General Public License v3 (GPL).

<http://www.gnu.org/licenses/gpl-3.0.en.html>

- We appreciate your citation of the following paper when you use the OpenMX Viewer for your research:

"OpenMX Viewer: A web-based crystalline and molecular graphical user interface program",  
Y.-T. Lee and T. Ozaki, Journal of Molecular Graphics and Modelling 89, 192-198 (2019).

<https://doi.org/10.1016/j.jmgm.2019.03.013>

# Release notes

## OpenMX Viewer:

Ver. 1.00: Aug. 19, 2016    Ver. 1.29: Feb. 16, 2020    Ver. 1.62: Feb. 15, 2026  
Ver. 1.01: Aug. 20, 2016    Ver. 1.30: Apr. 12, 2021    Ver. 1.63: Feb. 21, 2026  
Ver. 1.02: Aug. 30, 2016    Ver. 1.31: Jun. 18, 2022    Ver. 1.64: Feb. 22, 2026  
Ver. 1.05: Sep. 17, 2016    Ver. 1.36: Jul. 06, 2022    Ver. 1.65: Feb. 27, 2026  
Ver. 1.06: Oct. 21, 2016    Ver. 1.37: Jul. 10, 2022  
Ver. 1.07: Dec. 13, 2016    Ver. 1.38: Jul. 12, 2022  
Ver. 1.08: Dec. 27, 2016    Ver. 1.39: Jul. 16, 2022  
Ver. 1.09: Mar. 08, 2017    Ver. 1.40: Aug. 03, 2022  
Ver. 1.10: Apr. 08, 2017    Ver. 1.41: Aug. 07, 2022  
Ver. 1.11: Apr. 29, 2017    Ver. 1.42: Aug. 08, 2022  
Ver. 1.12: May 05, 2017    Ver. 1.43: Aug. 08, 2022  
Ver. 1.13: Dec. 08, 2017    Ver. 1.44: Aug. 09, 2022  
Ver. 1.14: Dec. 25, 2017    Ver. 1.45: Aug. 09, 2022  
Ver. 1.15: Dec. 25, 2017    Ver. 1.46: Aug. 09, 2022  
Ver. 1.16: Jan. 31, 2018    Ver. 1.47: Aug. 12, 2022  
Ver. 1.17: Feb. 06, 2018    Ver. 1.48: Sep. 20, 2022  
Ver. 1.18: Feb. 23, 2018    Ver. 1.49: Nov. 11, 2022  
Ver. 1.19: Feb. 24, 2018    Ver. 1.52: Feb. 01, 2023  
Ver. 1.20: Feb. 25, 2018    Ver. 1.53: Feb. 01, 2023  
Ver. 1.21: Feb. 25, 2018    Ver. 1.54: Feb. 10, 2023  
Ver. 1.22: Mar. 01, 2018    Ver. 1.55: Feb. 15, 2023  
Ver. 1.23: Mar. 05, 2018    Ver. 1.56: Jul. 15, 2023  
Ver. 1.24: Mar. 23, 2018    Ver. 1.57: Jul. 17, 2023  
Ver. 1.25: Sep. 09, 2019    Ver. 1.58: Mar. 06, 2025  
Ver. 1.26: Nov. 14, 2019    Ver. 1.59: Dec. 04, 2025  
Ver. 1.27: Nov. 14, 2019    Ver. 1.60: Dec. 05, 2025  
Ver. 1.28: Jan. 03, 2020    Ver. 1.61: Dec. 09, 2025

## Manual:

1<sup>st</sup> edition: Jul. 17, 2022  
2<sup>nd</sup> edition: Feb. 02, 2023  
3<sup>rd</sup> edition: Jul. 27, 2023  
4<sup>th</sup> edition: Dec. 06, 2025  
5<sup>th</sup> edition: Feb. 23, 2026  
6<sup>th</sup> edition: Feb. 27, 2026

# Web browsers we tested and recommended ones

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So far, we have tested the OpenMX Viewer on the following browsers:

Chrome, Edge, Firefox, Opera, Safari, Waterfox, Brave, Vivaldi, SRWare, Avast, and Sleipnir.

Our test (Dec. 06, 2025) suggests that the OpenMX Viewer can be used without stress on Chrome and Edge due to its performance.

We would like to recommend you the use of these Web browsers.

# Getting started with OpenMX Viewer

Visit the website: <http://www.openmx-square.org/viewer/> and drag & drop a dat, xyz, cube, md, or cif file on the site. Then, you will see the structure of your model.



Chrome or Edge is recommended due to its performance.

**Welcome to OpenMX Viewer**

Drag & drop here the following file:  
a dat, xyz, cube, md, or cif file

Reset Display Canvas2D  Supercell 1 × 1 × 1 Brillouin zone  Atoms rendering  Bonds rendering1  BGC  Bond Color  Number  Symbol  Atomic Attributes  Atom Size

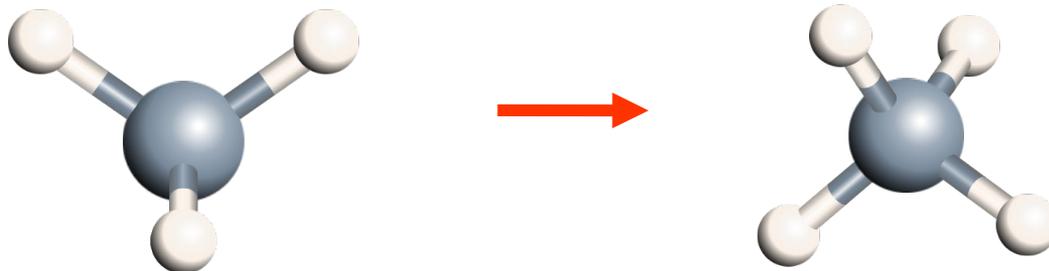
0.5 Bond Thickness 1.0 Bond Factor 1.05 Cells  Axes  Structure  Dynamics  Net Charge off  Spin off  Force  Velocity  Rot on a 0  Rot on b 0  Rot on c 0

Save  Save image Save config. Examples  Manual OpenMX website Reference Rotate: click+drag Zoom: scroll Translate: ctrl+click+drag

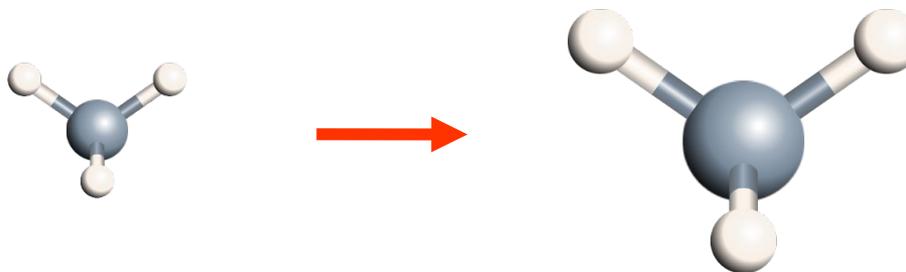
Here is the main control panel as we will explain in the next slides.

# Rotation, zooming, and translation

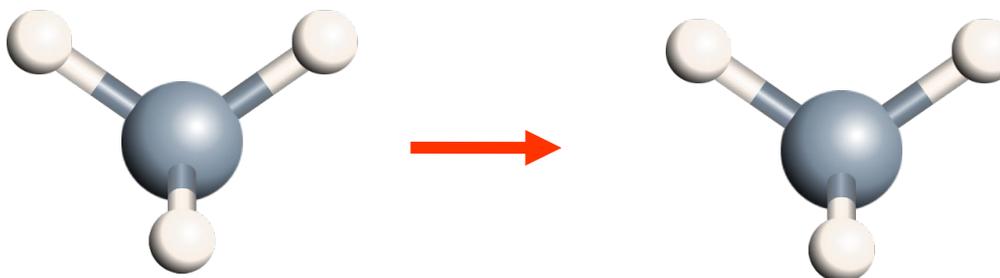
- You can rotate the structure by “click+drag”.



- You can zoom in and out the structure by “scroll”.



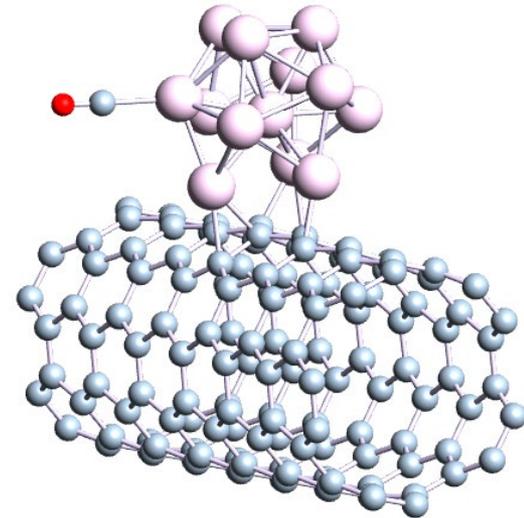
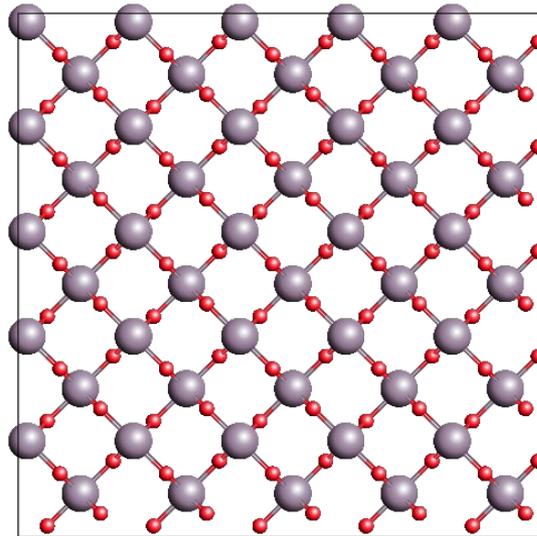
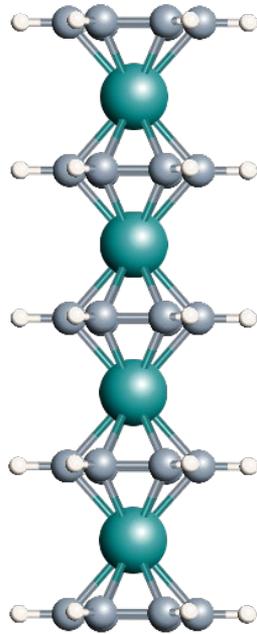
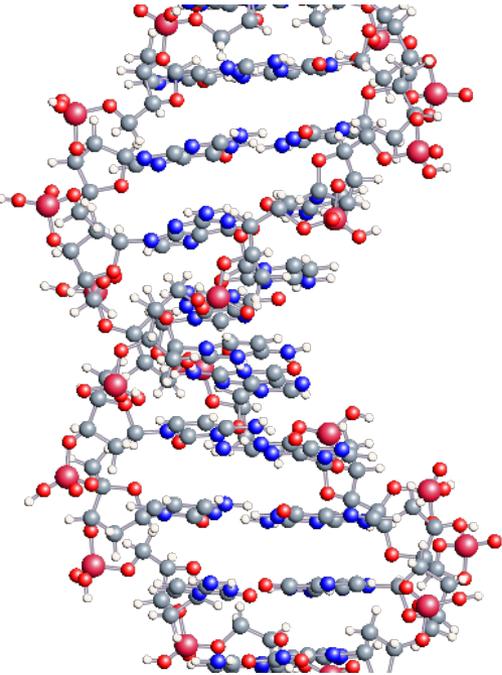
- You can translate the structure by “ctrl+click+drag”.



# Examples

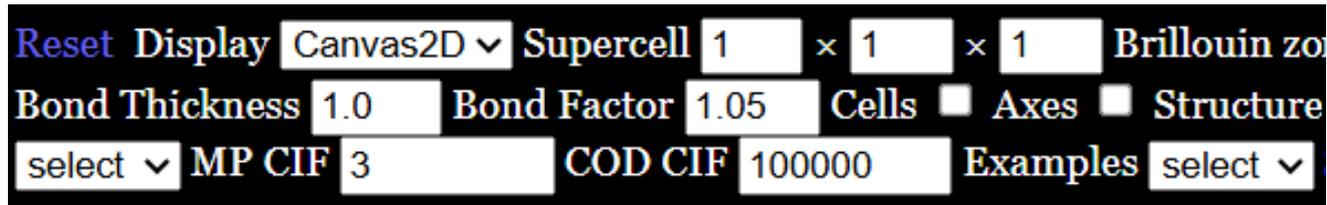
Examples

- Examples for the *xyz*, *cif*, *dat*, *md*, and *cube* files are selected by “Examples” as shown below.

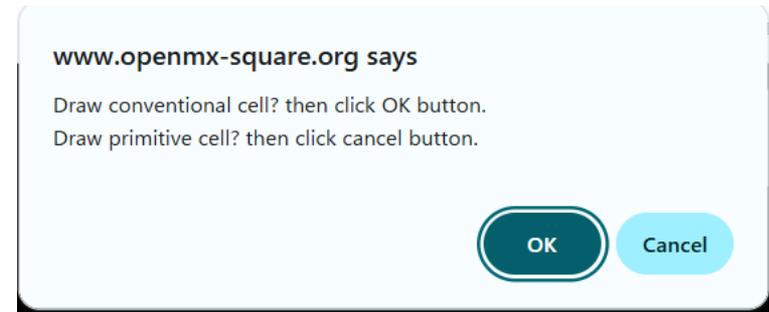


# Loading CIF from Materials Project

One can load a CIF from the Materials Project dataset (snapshot) hosted on the OpenMX Viewer server (downloaded Feb 22, 2026), which is licensed under CC BY 4.0.



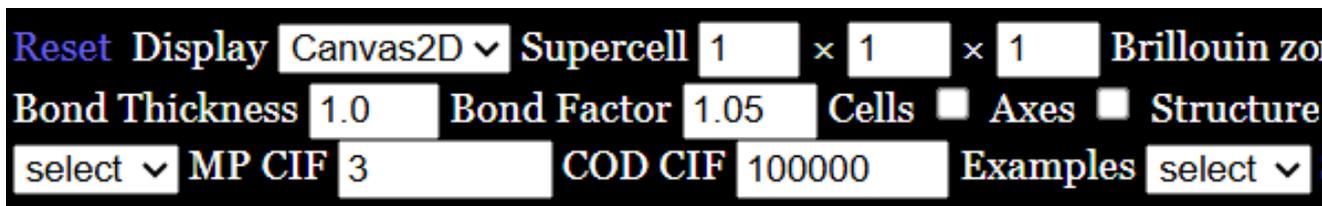
By just specifying the **Materials Project ID** in the MP CIF field, the corresponding CIF is automatically loaded from the OpenMX Viewer server and visualized as a crystal structure. In some cases, you may be asked to choose the conventional or primitive cell as shown in the right figure.



This streamlines early-stage materials exploration by eliminating manual file download and management, while keeping the data source clear and the workflow reproducible (shareable by ID).

# Loading CIF from COD

One can load a CIF smaller than 1MB from the Crystallography Open Database (COD) hosted on the OpenMX Viewer server (downloaded Feb 27, 2026). COD data are provided under CC0 1.0, and users should acknowledge the original authors of the structural data.

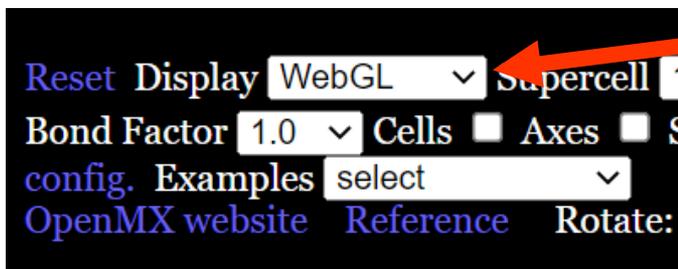


By specifying its **7-digit COD ID number** in the COD CIF field, the corresponding CIF is automatically loaded from the OpenMX Viewer server and visualized as a crystal structure. In some cases, you may be asked to choose the conventional or primitive cell as shown in the right figure.



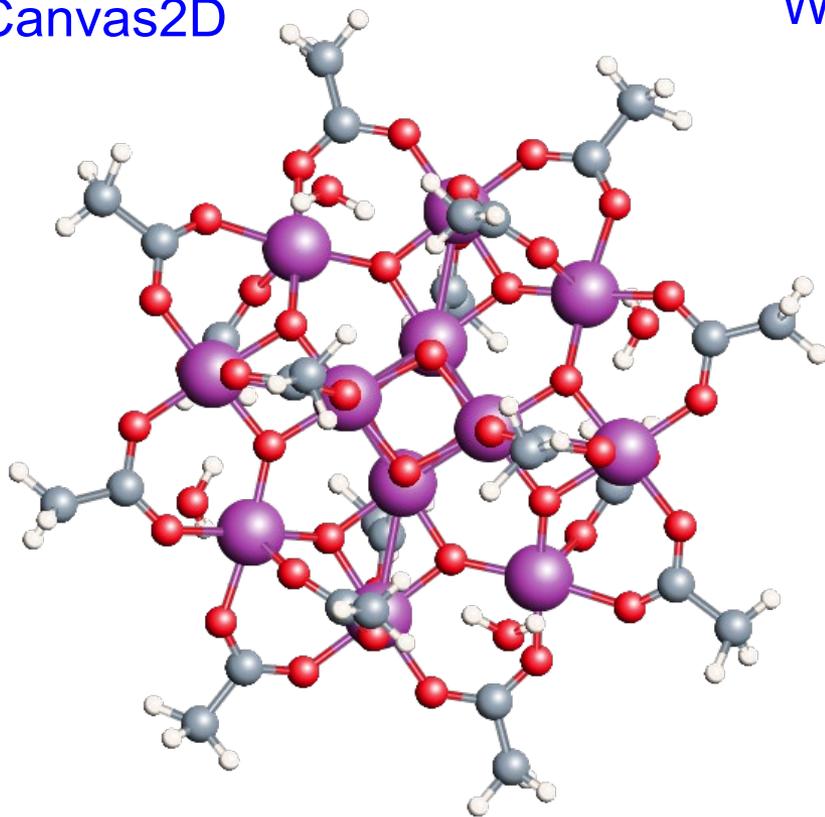
This allows quick inspection of a wide variety of structures without manually downloading CIF files. In some cases, you may be asked whether the conventional or primitive cell is selected.

# Canvas2D or WebGL

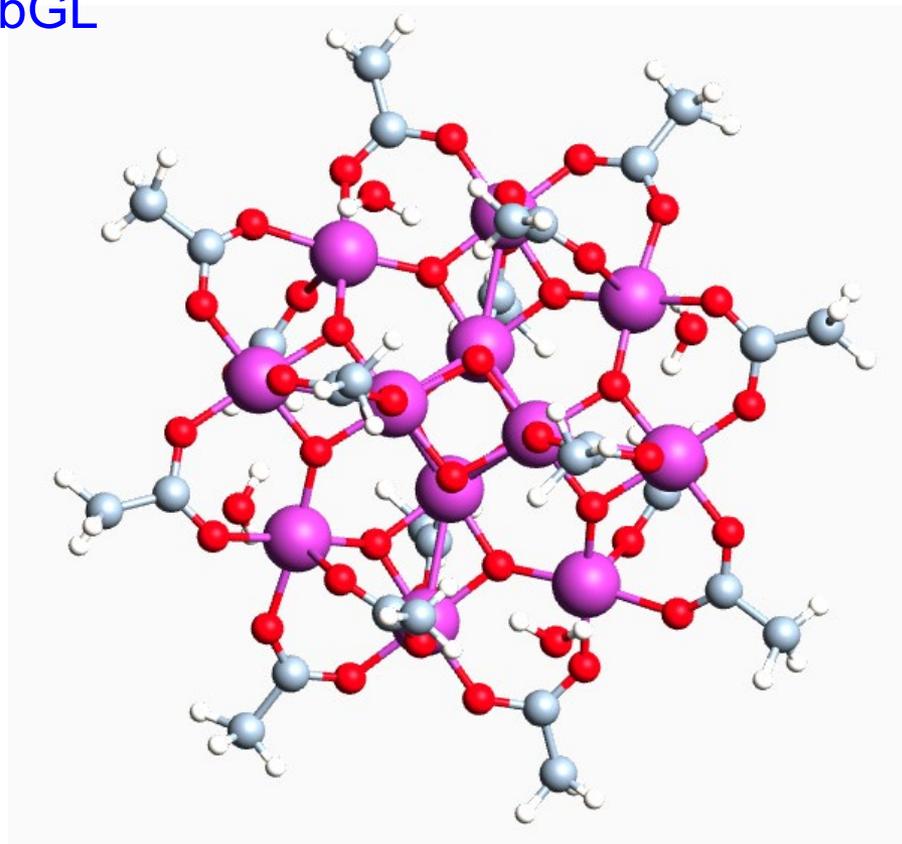


- The display style can be chosen as either Canvas2D or WebGL. The following is an example.

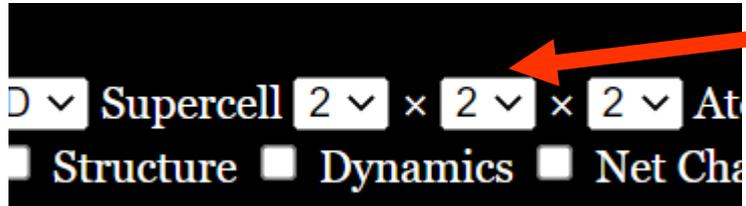
Canvas2D



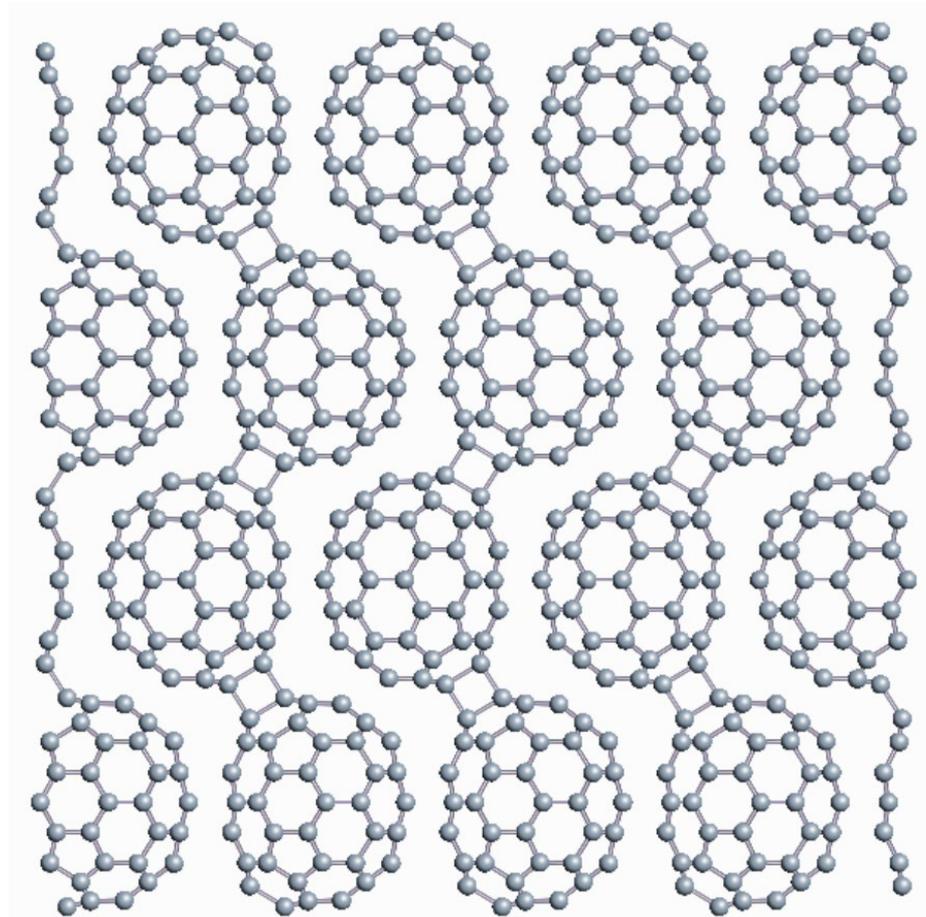
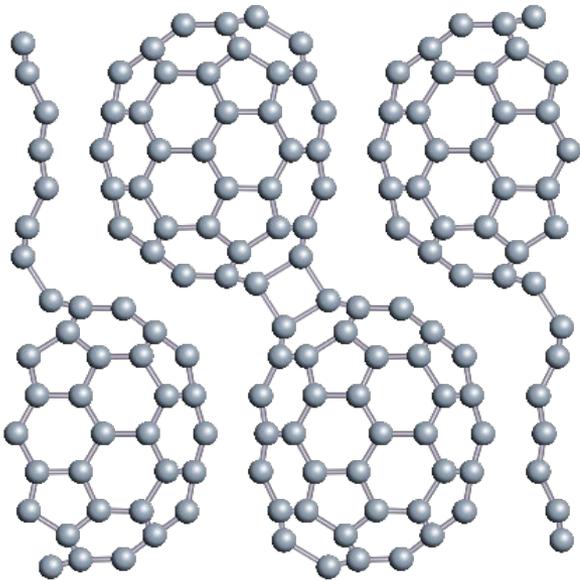
WebGL



# Supercell



- The supercell can be easily generated by selecting the number of cells along a-, b-, and c-axes.



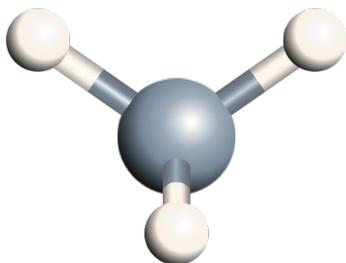
# Display style of atoms and bonds

Atoms rendering ▾ Bonds rendering1 ▾

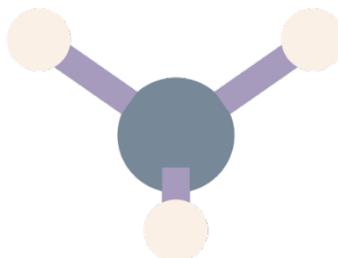
- The display styles of atoms and bonds are controlled by “Atoms” and “Bonds”. The followings are examples.

## ■ Canvas2D

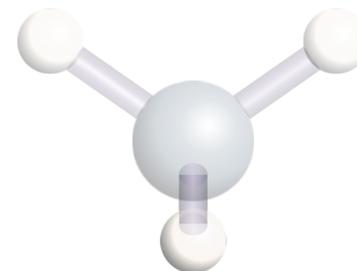
*rendering1*



*solid+wire*

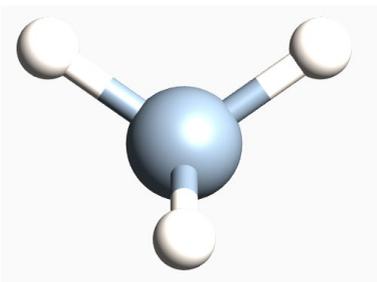


*translucent*

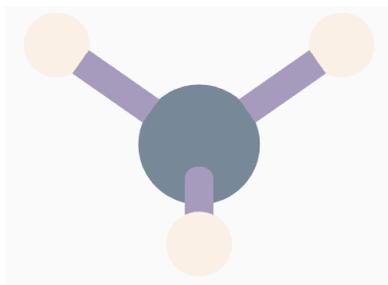


## ■ WebGL

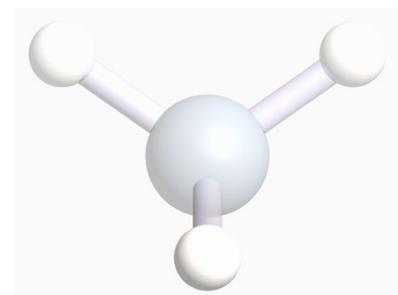
*rendering1*



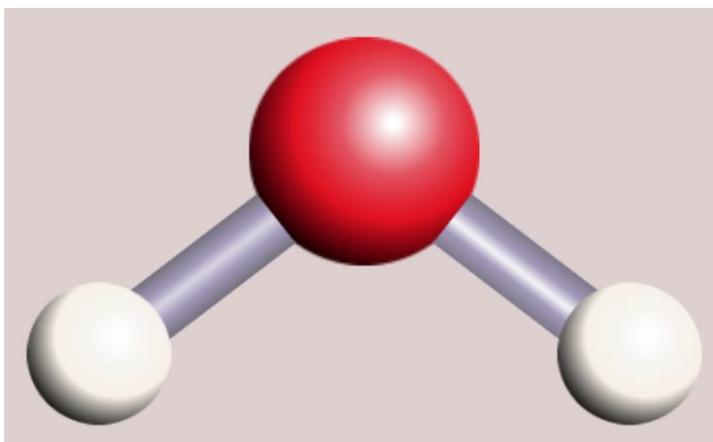
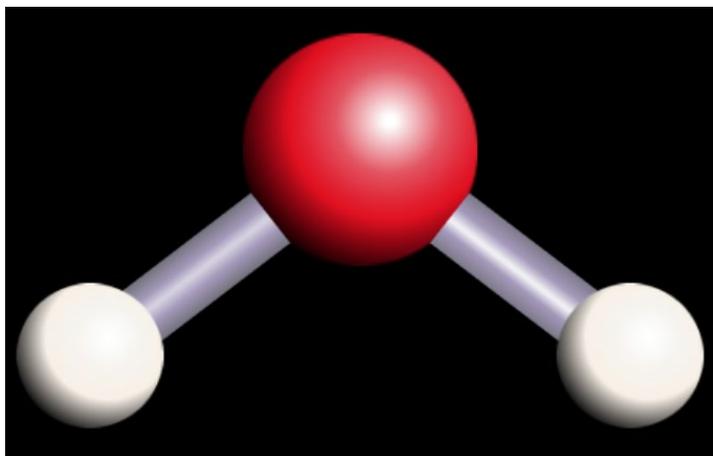
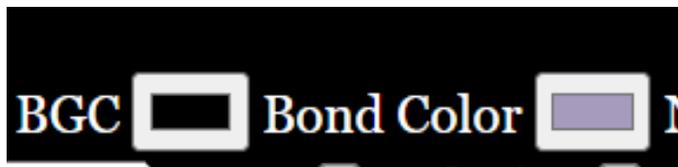
*solid+wire*



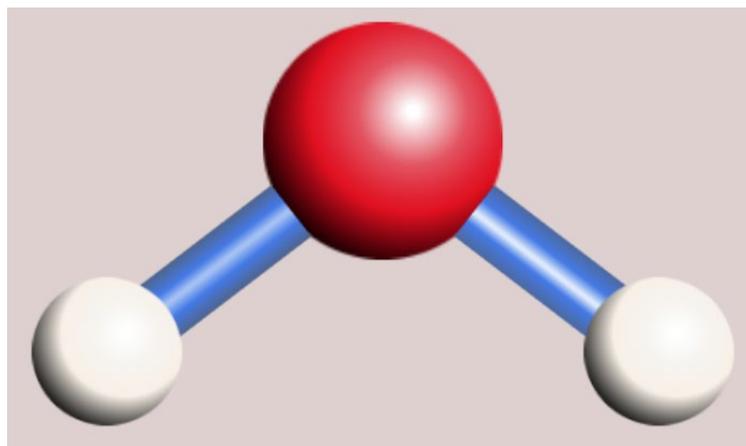
*translucent*



# Background and bond colors



- The color of background can be changed by “BGC”, and the color of bonds can be controlled by “Bond Color” when “Bonds=rendering2” as shown below:

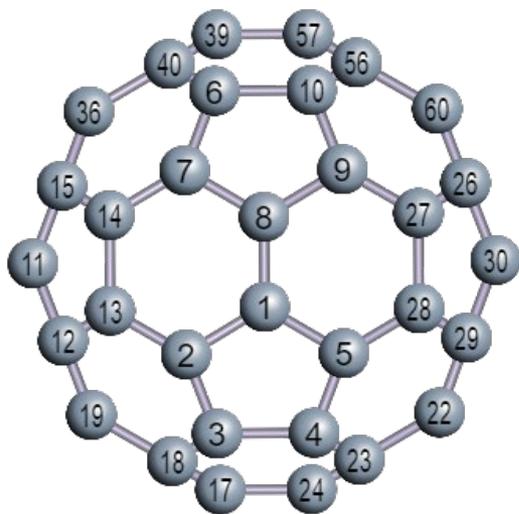


# Displaying atomic serial number and symbol

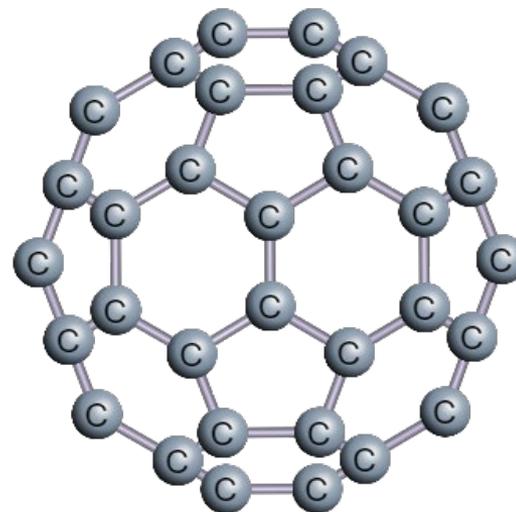
Number  Symbol

- The serial number of atoms, atomic symbol, and both of them can be displayed by checking “Number” or/and “Symbol”.

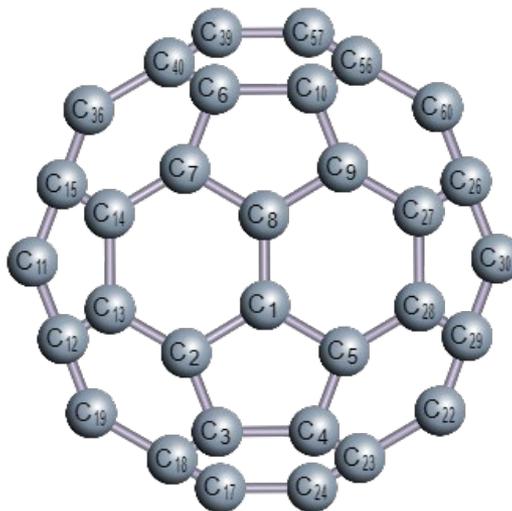
*Number checked*



*Symbol checked*



*Number and Symbol checked*



# Atomic Attributes #1

## Atomic Attributes

Attributes of atoms can be changed by checking “Atomic Attributes”. You will see the following a periodic table. By clicking one of elements, a small control panel pops up as shown below.

**6: C** X

Atomic radius  X

Color

Basis set

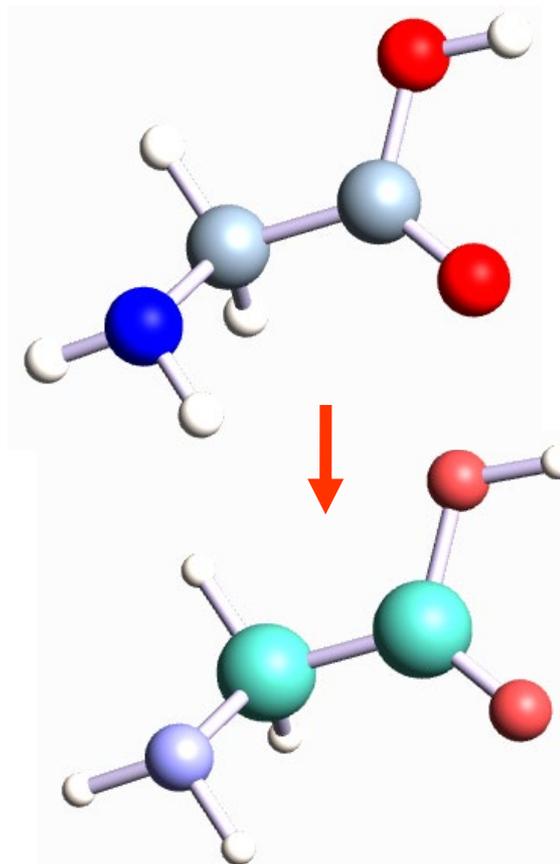
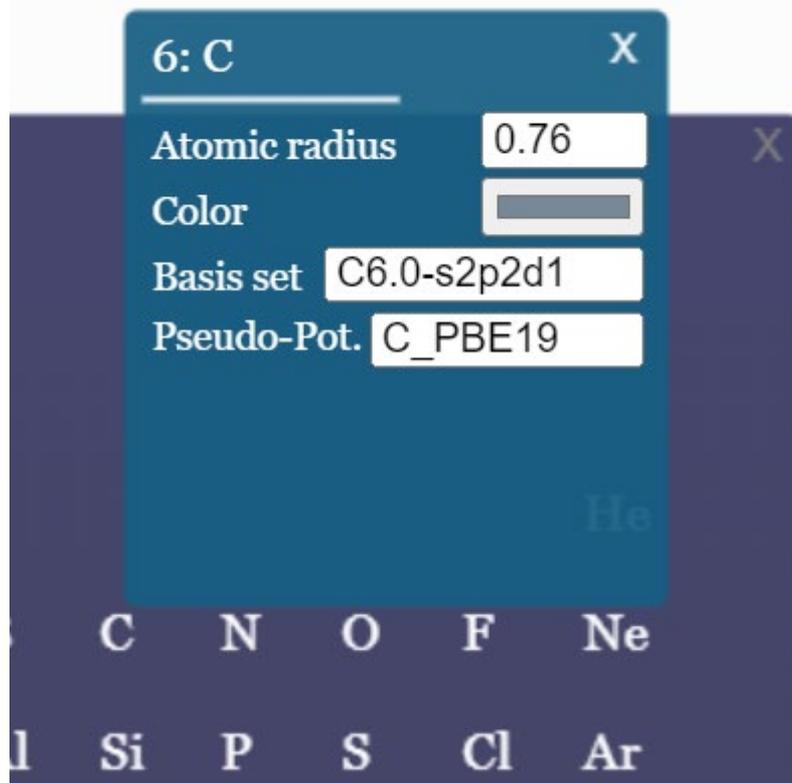
Pseudo-Pot.

**Periodic Table**

E																			
H																			He
Li	Be										B	C	N	O	F	Ne			
Na	Mg										Al	Si	P	S	Cl	Ar			
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	A																	
	L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
	A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

# Atomic Attributes #2

- The radius, color, basis set, and pseudopotential of each element can be changed in the control panel. By changing the radii and colors of elements, one can obtain a proper visualization depending on your sense. The following is an example. The setting of basis set and pseudopotential will be reflected in generating the input file. To close the control panel, push “X”.



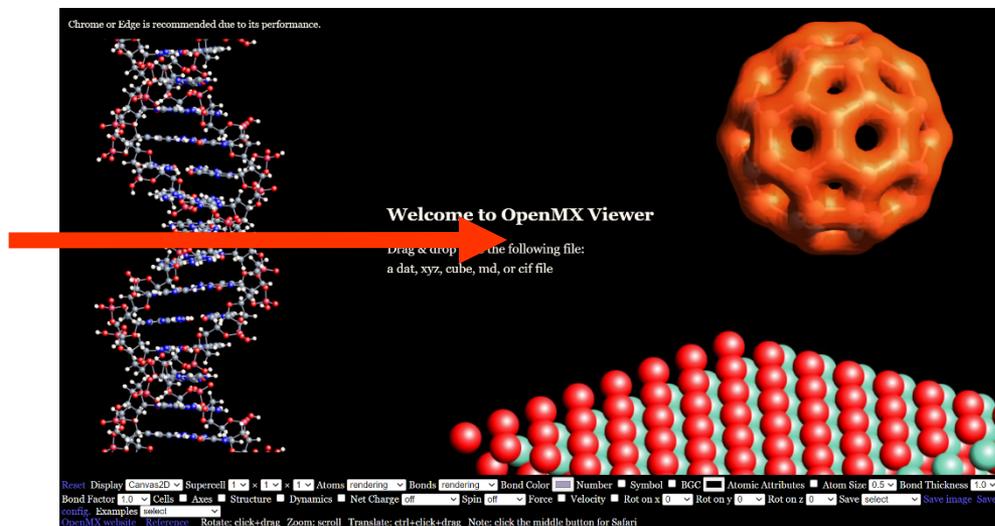
# Atomic Attributes #3



- The settings by the control panel including the periodic table panel can be saved to a configuration file by clicking “Save config.”.

- In the next use, you can start with the configuration by dragging and dropping it onto the website of the OpenMX Viewer.

- Just drag&drop “omxv.config” onto the web to start with your configuration.

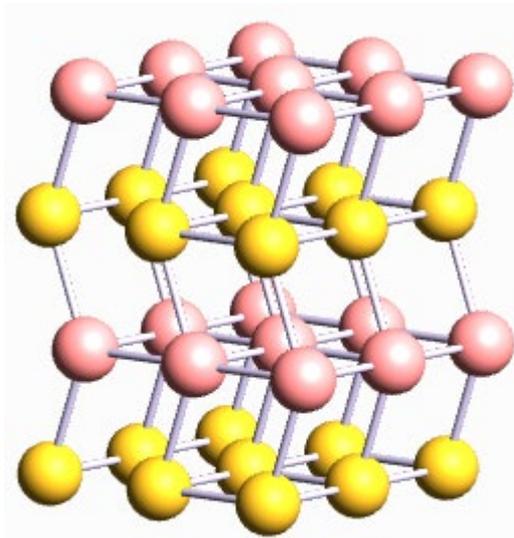


# Atom Size and Bond Thickness

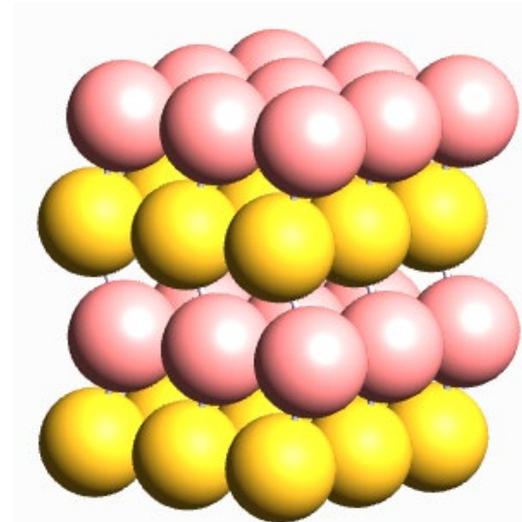
Atom Size  Bond Thickness

- The scaling factors for atomic radii and bond thickness are controlled by setting “Atom Size” and “Bond Thickness”, respectively, where the default values are set to 0.5 and 1.0, respectively. The following is an example.

Default



*Atom Size = 1.0*

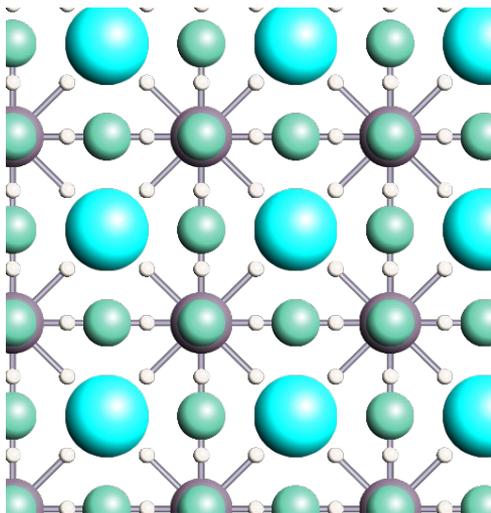


# Bond Factor

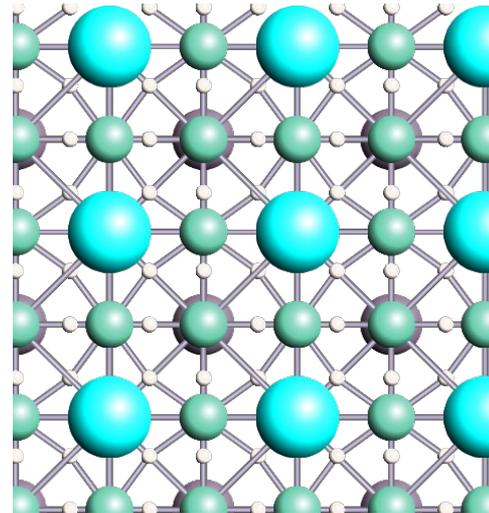
Bond Factor 1.0 ▼

- As default, a bond is generated if the distance between two atoms is smaller than the sum of atomic radii.
- The threshold is changed by “Bond Factor” so that the bond can be formed if the distance between two atoms is smaller than the sum of atomic radii times the value of “Bond Factor”. Note that the default value is 1. The following is an example.

Default



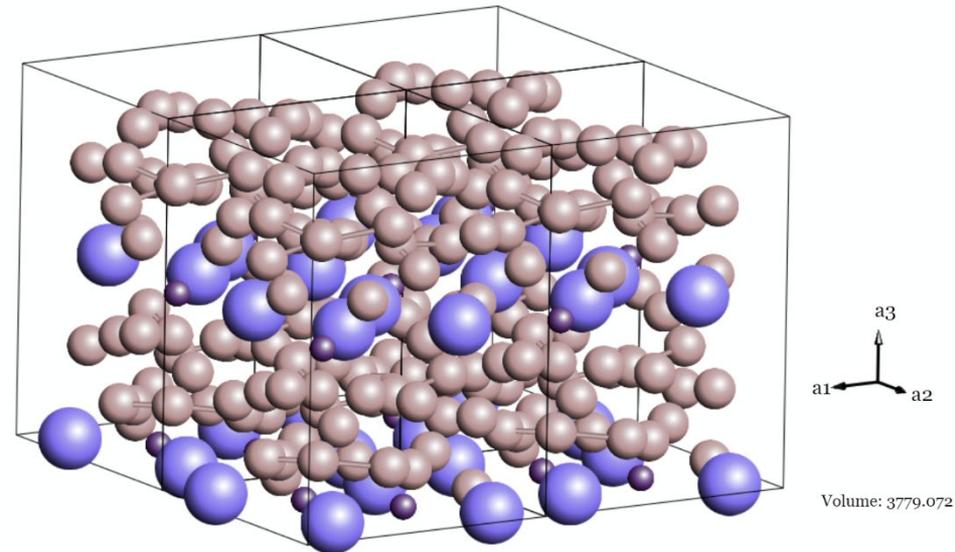
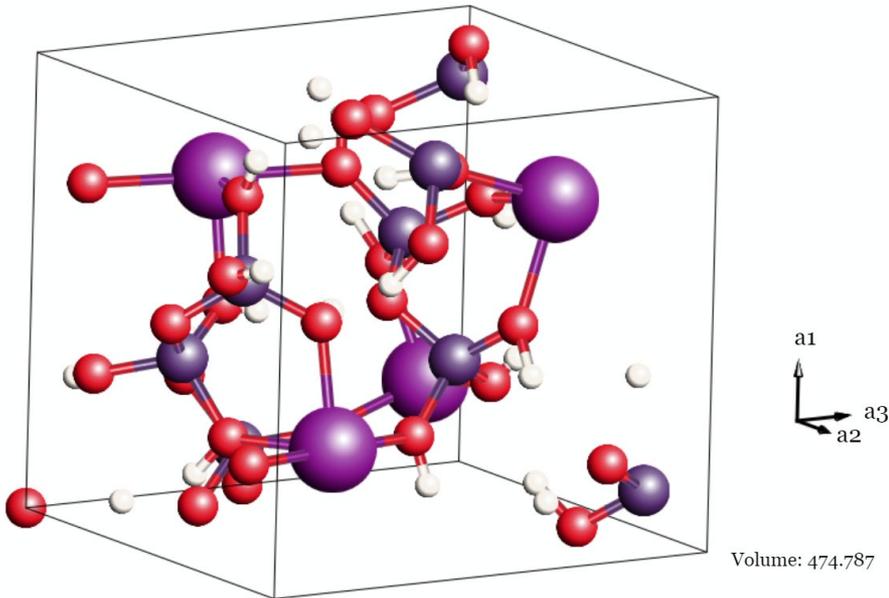
*Bond Factor = 1.1*



# Cells and Axes

Cells  Axes

- The unit cells and axes are displayed by checking “Cells” and “Axes”, respectively. The followings are examples.

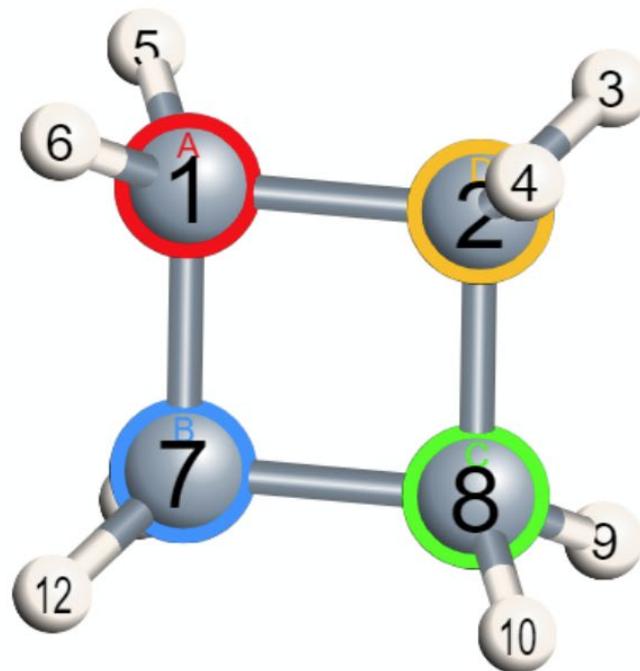


# Analysis of Structure

**Structure**

- The structure such as bond length and bond angle can be analyzed by clicking “Structure”. Then, a control panel pops up as shown below.
- Clicking atoms marks selected atoms with colored circles, and the bond length, angles, and dihedral angle are shown in the control panel. The position of the control panel can be moved by hanging “Analysis of Structure”.
- To close the control panel, push “X”.

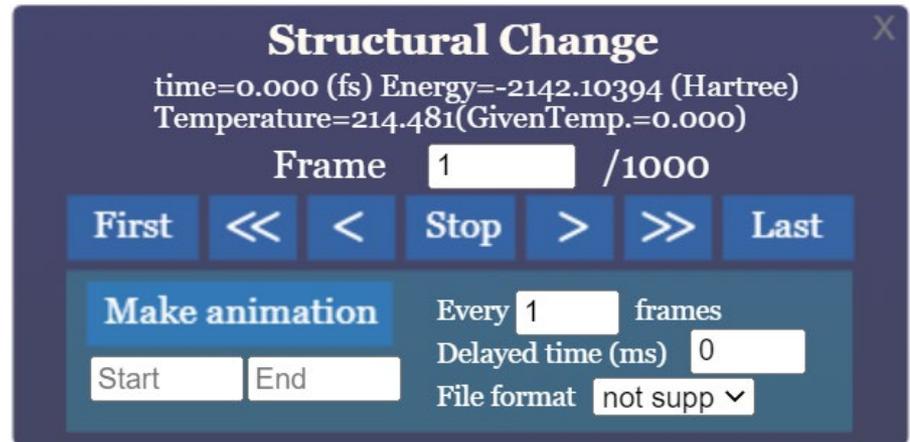
Analysis of Structure			
	x (Ang.)	y (Ang.)	z (Ang.)
A=C 1 (1,0,0,0)	-0.7776	+0.0000	-0.7773
B=C 7 (7,0,0,0)	-0.7776	+0.0000	+0.7773
C=C 8 (8,0,0,0)	+0.7768	+0.0000	+0.7773
D=C 2 (2,0,0,0)	+0.7768	+0.0000	-0.7773
<b>Length:</b>	AB=1.5546	BC=1.5544	CD=1.5546
<b>Angle:</b>	ABC=90.00	BCD=90.00	
<b>Dihedral Angle:</b>	ABCD=0.00		
Length in Ang. Angle in Deg.			



# Animation for *xyz* and *md* files

## Dynamics

- The xyz and md files can be animated by checking “Dynamics”. In this case, you will see a control panel as



- By pushing “<” and “>”, the frame of structures goes backward and forward, respectively.
- By “<<” and “>>”, the structure is animated towards backward and forward direction, respectively. Pushing “<<” and “>>” several times accelerates the display speed.
- The functionality of “Make animation” is not supported yet. So, please use a capture software to create video files. As for the format of md file, please see the next slide.

# Format of the *md* file #1

- The *md* file, supported by OpenMX, is an extension of the xyz file, and the format is as follows:

1st step

```

10
time= 0.000 (fs) Energy= -56.61840 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041 0.00000 0.00000 0.00000 10.18041 0.00000 0.00000 0.00000 8.55154
C -0.55502 -0.05167 0.35409 0.03654 -0.00779 -0.03763 -1394.21538 338.60117 -141.80824 -0.49099 0.00000 0.00000 0.00000
C 0.81500 -0.46585 -0.13783 -0.18935 -0.00202 0.02830 992.13064 -1040.97544 103.16876 0.07147 0.00000 0.00000 0.00000
O 0.86860 -1.67958 -0.73136 -0.14908 -0.15936 -0.04402 897.25381 825.75866 269.26108 -0.58253 0.00000 0.00000 0.00000
N -0.89697 1.28481 -0.17674 -0.00318 -0.04569 -0.07022 670.45601 -1105.81277 330.04574 -0.64593 0.00000 0.00000 0.00000
H -1.33580 -0.76012 0.00834 -0.03932 -0.04284 -0.01955 -3662.52988 -1946.83894 -2746.85085 0.20500 0.00000 0.00000 0.00000
H -0.54756 -0.10941 1.46450 -0.00875 0.00561 0.08037 3224.74855 -3639.73773 -1050.14409 0.15894 0.00000 0.00000 0.00000
O 1.87095 0.13365 -0.04595 0.24840 0.16347 0.03671 -629.69966 -665.38792 848.63451 -0.57897 0.00000 0.00000 0.00000
H 1.75863 -1.86736 -1.01311 0.11935 -0.01038 -0.03189 -3177.81107 145.86589 3824.88386 0.34050 0.00000 0.00000 0.00000
H -1.77844 1.56501 0.19676 -0.09529 0.03530 0.03816 2071.02647 -3750.21792 2529.07325 0.24358 0.00000 0.00000 0.00000
H -0.19940 1.95052 0.08130 0.07811 0.06151 0.02131 255.20767 -67.42941 4967.87871 0.27892 0.00000 0.00000 0.00000

```

2nd step

```

10
time= 0.200 (fs) Energy= -56.61485 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041 0.00000 0.00000 0.00000 10.18041 0.00000 0.00000 0.00000 8.55154
C -0.55777 -0.05100 0.35377 0.03487 -0.01511 -0.04015 -1394.21538 338.60117 -141.80824 -0.48748 0.00000 0.00000 0.00000
C 0.81683 -0.46794 -0.13760 -0.19595 -0.00079 0.02998 992.13064 -1040.97544 103.16876 0.07137 0.00000 0.00000 0.00000
O 0.87030 -1.67803 -0.73085 -0.15944 -0.15994 -0.04333 897.25381 825.75866 269.26108 -0.58701 0.00000 0.00000 0.00000
N -0.89564 1.28257 -0.17613 0.00130 -0.04063 -0.07086 670.45601 -1105.81277 330.04574 -0.64508 0.00000 0.00000 0.00000
H -1.34350 -0.76443 0.00265 -0.03445 -0.03836 -0.01723 -3662.52988 -1946.83894 -2746.85085 0.20217 0.00000 0.00000 0.00000
H -0.54120 -0.11663 1.46319 -0.00903 0.00540 0.08059 3224.74855 -3639.73773 -1050.14409 0.15931 0.00000 0.00000 0.00000
O 1.86985 0.13242 -0.04423 0.25269 0.16668 0.03755 -629.69966 -665.38792 848.63451 -0.58053 0.00000 0.00000 0.00000
H 1.75346 -1.86717 -1.00578 0.13010 -0.01354 -0.03481 -3177.81107 145.86589 3824.88386 0.34479 0.00000 0.00000 0.00000
H -1.77523 1.55786 0.20219 -0.09718 0.03597 0.03909 2071.02647 -3750.21792 2529.07325 0.24466 0.00000 0.00000 0.00000
H -0.19812 1.95100 0.09144 0.07457 0.05823 0.02067 255.20767 -67.42941 4967.87871 0.27779 0.00000 0.00000 0.00000

```

```

10
time= 0.400 (fs) Energy= -56.61317 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041 0.00000 0.00000 0.00000 10.18041 0.00000 0.00000 0.00000 8.55154
C -0.56059 -0.05034 0.35337 0.03267 -0.02305 -0.04150 -1422.28190 339.93279 -182.46142 -0.48282 0.00000 0.00000 0.00000
C 0.81840 -0.47011 -0.13730 -0.20117 0.00108 0.03168 865.04417 -1085.02515 133.18142 0.07108 0.00000 0.00000 0.00000
O 0.87187 -1.67661 -0.73037 -0.16673 -0.16130 -0.04381 831.90187 757.06130 252.42603 -0.59010 0.00000 0.00000 0.00000

```

.....

- Each block of data corresponds to each structural step as shown above, and the format of each block will be explained in the next slide.

# Format of the *md* file #2

- Each block of the *md* file has the following format:

```

10
time= 0.000 (fs) Energy= -56.61840 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041 0.00000 0.00000 0.00000 10.18041 0.00000 0.00000 0.00000 8.55154
C -0.55502 -0.05167 0.35409 0.03654 -0.00779 -0.03763 -1394.21538 338.60117 -141.80824 -0.49099 0.00000 0.00000 0.00000
C 0.81500 -0.46585 -0.13783 -0.18935 -0.00202 0.02830 992.13064 -1040.97544 103.16876 0.07147 0.00000 0.00000 0.00000
O 0.86860 -1.67958 -0.73136 -0.14908 -0.15936 -0.04402 897.25381 825.75866 269.26108 -0.58253 0.00000 0.00000 0.00000
N -0.89697 1.28481 -0.17674 -0.00318 -0.04569 -0.07022 670.45601 -1105.81277 330.04574 -0.64593 0.00000 0.00000 0.00000
H -1.33580 -0.76012 0.00834 -0.03932 -0.04284 -0.01955 -3662.52988 -1946.83894 -2746.85085 0.20500 0.00000 0.00000 0.00000
H -0.54756 -0.10941 1.46450 -0.00875 0.00561 0.08037 3224.74855 -3639.73773 -1050.14409 0.15894 0.00000 0.00000 0.00000
O 1.87095 0.13365 -0.04595 0.24840 0.16347 0.03671 -629.69966 -665.38792 848.63451 -0.57897 0.00000 0.00000 0.00000
H 1.75863 -1.86736 -1.01311 0.11935 -0.01038 -0.03189 -3177.81107 145.86589 3824.88386 0.34050 0.00000 0.00000 0.00000
H -1.77844 1.56501 0.19676 -0.09529 0.03530 0.03816 2071.02647 -3750.21792 2529.07325 0.24358 0.00000 0.00000 0.00000
H -0.19940 1.95052 0.08130 0.07811 0.06151 0.02131 255.20767 -67.42941 4967.87871 0.27892 0.00000 0.00000 0.00000

```

- Each line in each block corresponds to the following information:

**1<sup>st</sup> line:** the number of atoms

**2<sup>nd</sup> line:** The text before “Cell\_Vectors=..” is a comment. The “Cell\_Vectors=” is a keyword to provide cell vectors, **a**, **b**, **c**. They are arranged as  $a_x$ ,  $a_y$ ,  $a_z$ ,  $b_x$ ,  $b_y$ ,  $b_z$ ,  $c_x$ ,  $c_y$ , and  $c_z$  in Angstrom unit.

**3rd to the last lines:**

atomic symbol, x-, y-, z-coordinates in Angstrom unit, x-, y-, z-components of force in Hartree/Bohr, x-, y-, z-components of velocity in m/sec., net charge (electron charge is defined to be negative), local magnetic moment in Bohr magneton, Euler angles of spin in degree.

- An animated xyz file has a similar format, but the *md* file includes **the information of cell vectors** explicitly.

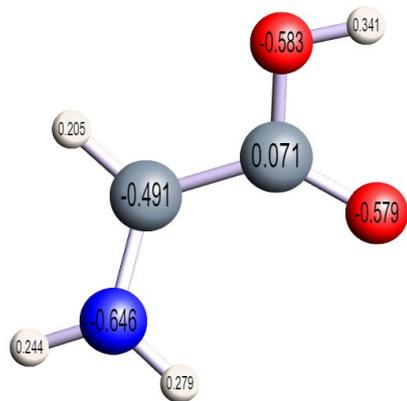
# Net charge and Spin

- The information of net charge and spin stored in a md file can be analyzed by “Net Charge” and “Spin”, respectively.

Net Charge Mulliken ▾ Spin off ▾

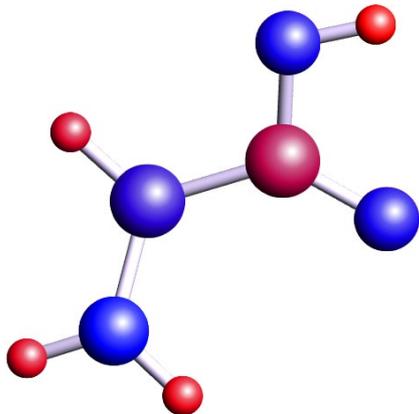
- The followings are examples.

Net Charge = Mulliken



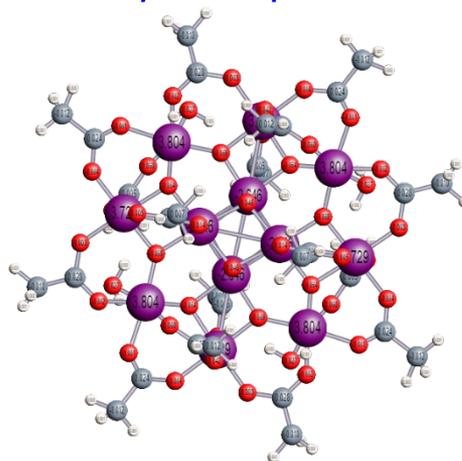
The net charge calculated by Mulliken population is shown on each atom, where zero means the neutral.

Net Charge = Mulliken-C



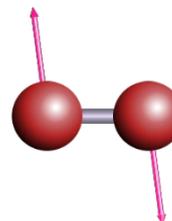
The net charge calculated by Mulliken population is shown by color, where the red and blue colors correspond to positive and negative, respectively.

Spin = spin



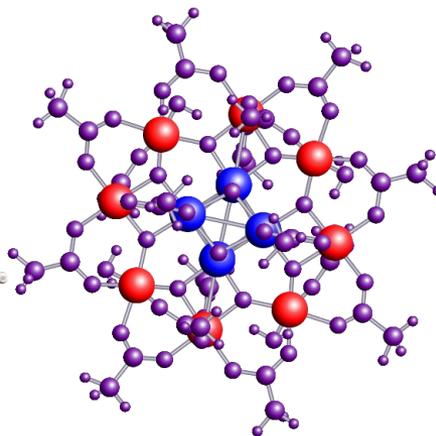
The local spin moment of each atom is shown in Bohr magneton.

Spin = spin-V



The non-collinear local spin moment of each atom is shown by a vector style.

Spin = spin-C

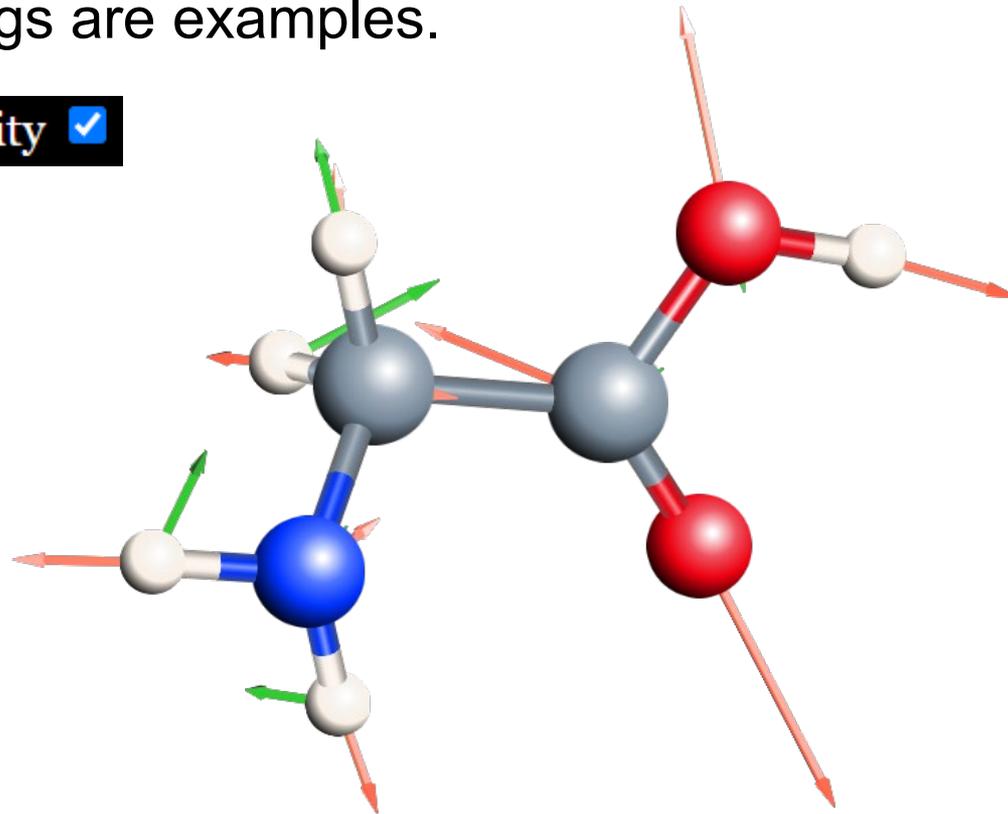


The local spin moment of each atom is shown by color, where the red and blue colors correspond to up- and down spin states, respectively.

# Force and Velocity

- The information of force and velocity stored in a md file can be analyzed by checking “Force” and “Velocity”, respectively. The followings are examples.

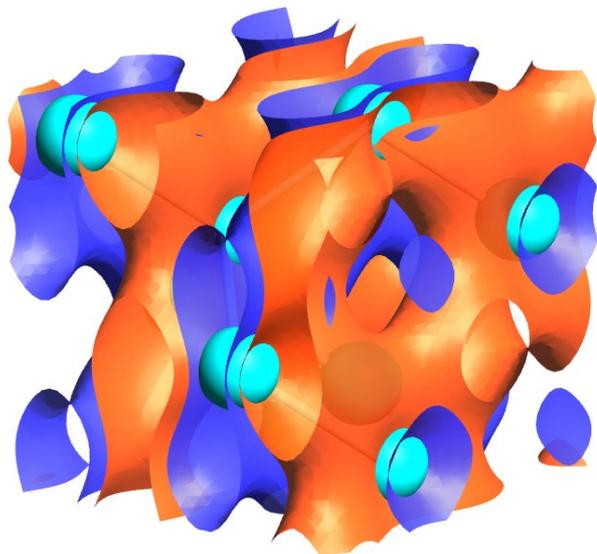
Force  Velocity



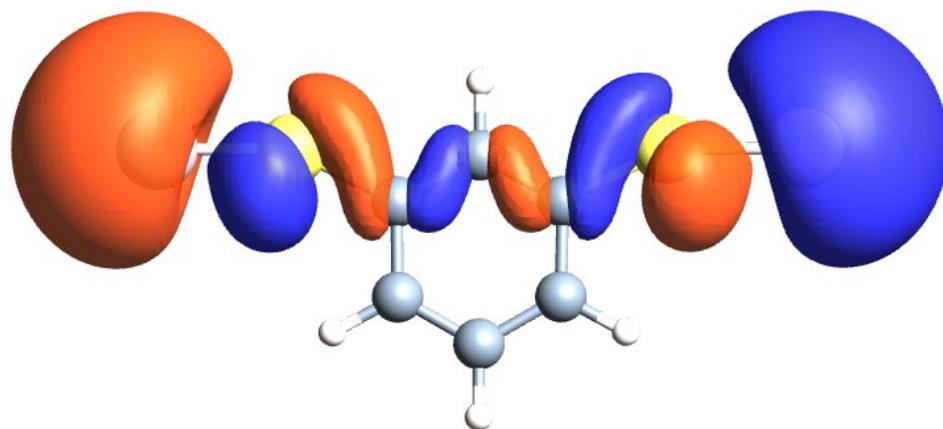
- The red and green arrows correspond to the force and velocity, respectively.

# Visualization of cube files

- By dragging and dropping a cube file onto the web, one can visualize isosurfaces as shown below.



- On a control panel appearing the right top, one can select an algorithm such as marching cubes to calculate the isosurface, and control parameters such as isovalue, opacity, and color.



Algorithm	Marching Cubes	▼
Isovalue	<input type="range"/>	0.016
Opacity	<input type="range"/>	0.9
Facets	<input checked="" type="checkbox"/>	
Edges	<input type="checkbox"/>	
Positive_Isosurface	<input checked="" type="checkbox"/>	
Negative_Isosurface	<input checked="" type="checkbox"/>	
Color_Positive	0xf04410	
Color_Negative	0x3333ff	
Close Controls		

# Visualization of 1<sup>st</sup> Brillouin zone

## Brillouin zone

The 1<sup>st</sup> Brillouin zone is shown by checking “Brillouin zone”, and a suggested k-path is also depicted by the red lines for the band structure calculation. By clicking “Suggested k-path”, you can download the k-path to a file. Also, the k-path will be included when you save an OpenMX input file. The generation of k-path is based on a paper: W. Setyawan and S. Curtarolo, *Comp. Mat. Sci.* 49, 299 (2010).

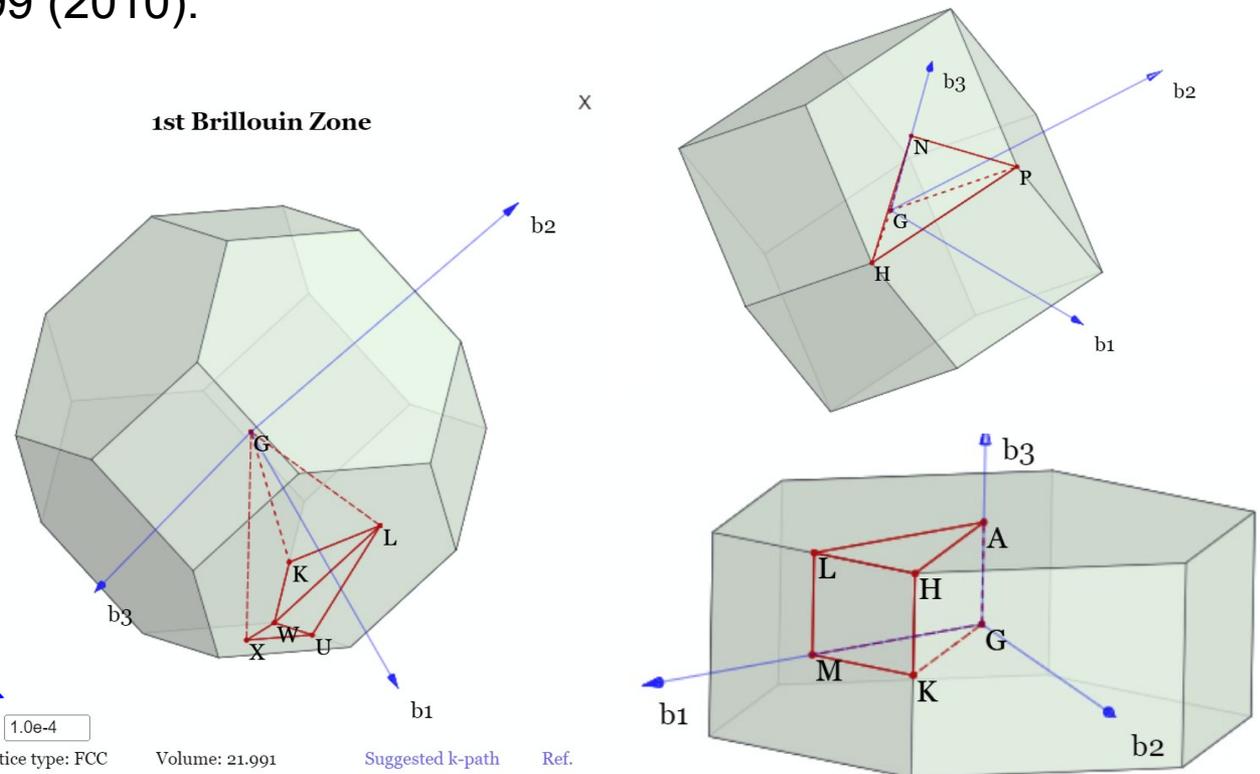
A common value is used to determine the Bravais lattice as tolerance of the length (Ang.) and angle (Deg.) of lattice vectors, which is controlled by “Tolerance”.

Tolerance   
Bravais lattice type: FCC

Volume: 21.991

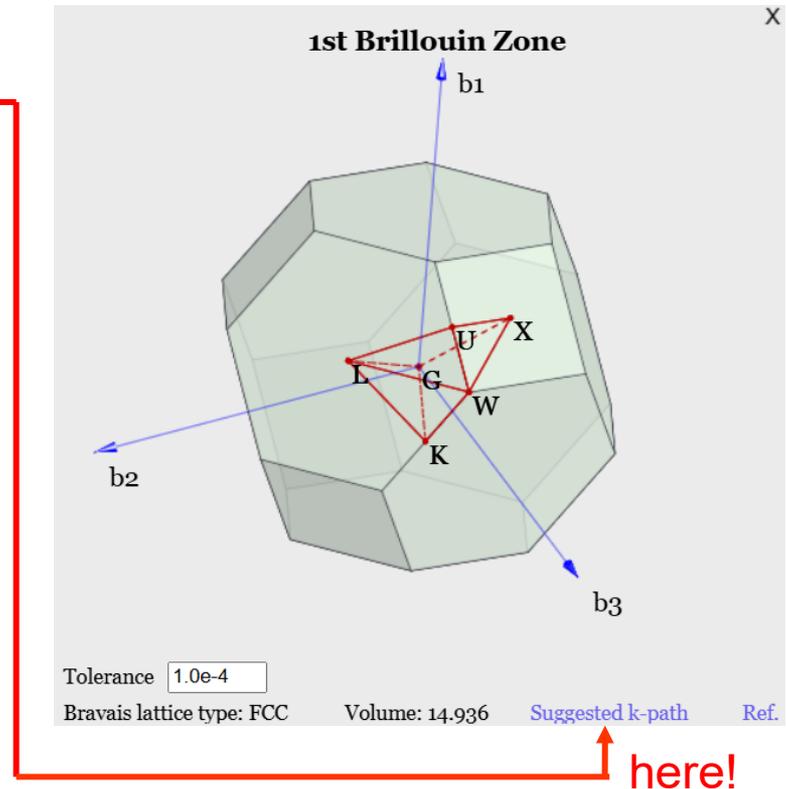
[Suggested k-path](#)

[Ref.](#)



# Automatic k-path generation

- After loading a crystal structure, simply click the “Suggested k-path” button.
- OpenMX Viewer analyzes the symmetry and builds a standard band-structure path through high-symmetry k-points; ref., W. Setyawan and S. Curtarolo, *Comp. Mat. Sci.* 49, 299 (2010).
- A file *kpath.txt* is automatically downloaded, containing the k-point labels, coordinates, and path segments for band calculations.
- This one-click workflow removes manual k-point lookup and makes it easy for you to obtain a reasonable k-path directly in the web browser.



k-path given in *kpath.txt*

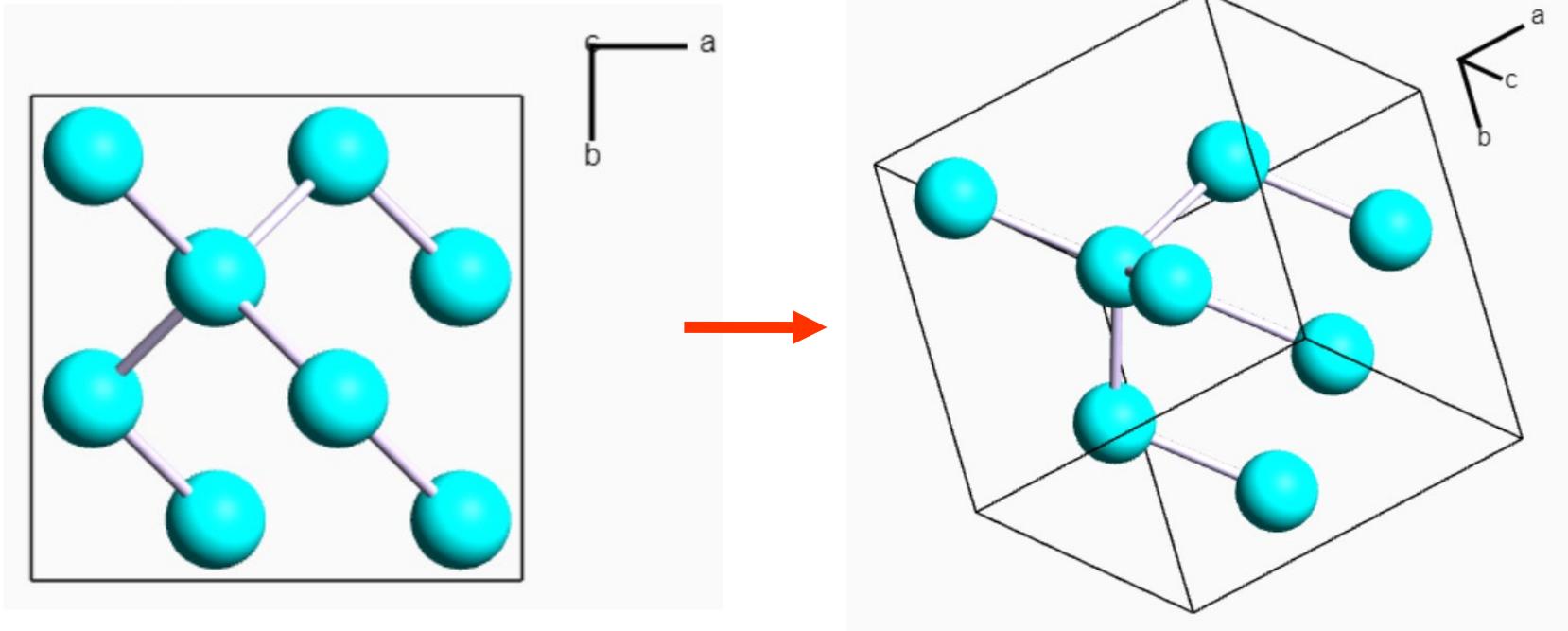
```
Band.Nkpath      10
<Band.kpath
 41 0.000000 0.000000 0.000000 0.500000 0.000000 0.500000 G X
 20 0.500000 0.000000 0.500000 0.500000 0.250000 0.750000 X W
 14 0.500000 0.250000 0.750000 0.375000 0.375000 0.750000 W K
 43 0.375000 0.375000 0.750000 0.000000 0.000000 0.000000 K G
 35 0.000000 0.000000 0.000000 0.500000 0.500000 0.500000 G L
 25 0.500000 0.500000 0.500000 0.625000 0.250000 0.625000 L U
 14 0.625000 0.250000 0.625000 0.500000 0.250000 0.750000 U W
 29 0.500000 0.250000 0.750000 0.500000 0.500000 0.500000 W L
 25 0.500000 0.500000 0.500000 0.375000 0.375000 0.750000 L K
 14 0.625000 0.250000 0.625000 0.500000 0.000000 0.500000 U X
Band.kpath>
```

# Rot on a-, b-, or c-axis

Rot on a  Rot on b  Rot on c

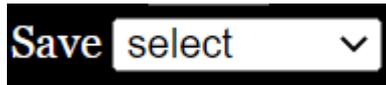
- The specific rotations of the structure can be performed by “Rot on a”, “Rot on b”, or “Rot on c” for on a-, b-, or c-axis, respectively. The following is an example.

Rotation on b-axis with 30 degree and then rotation on a-axis with 30 degree



# Saving xyz, cif, and OpenMX input files

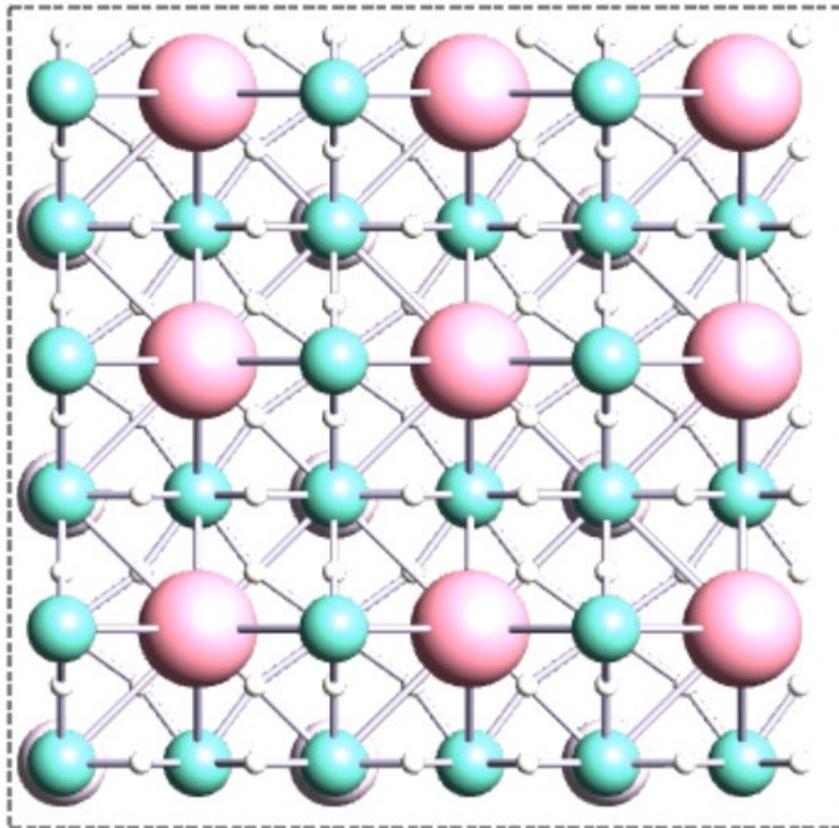
---



- You can save the structure as a *xyz*, *cif*, or OpenMX input files (*dat* file) by “Save”.
- By selecting one of the formats, a file is automatically saved as *abc.(xyz, cif, or dat)*. The *dat* file can be saved with either *xyz* or fractional coordinates, and setting the basis sets and pseudopotential can be done through “Atomic Attributes”.
- The *dat* files can be used as the input files for OpenMX calculations.
- Also, note that the input file for a supercell can be easily generated.

# Saving image

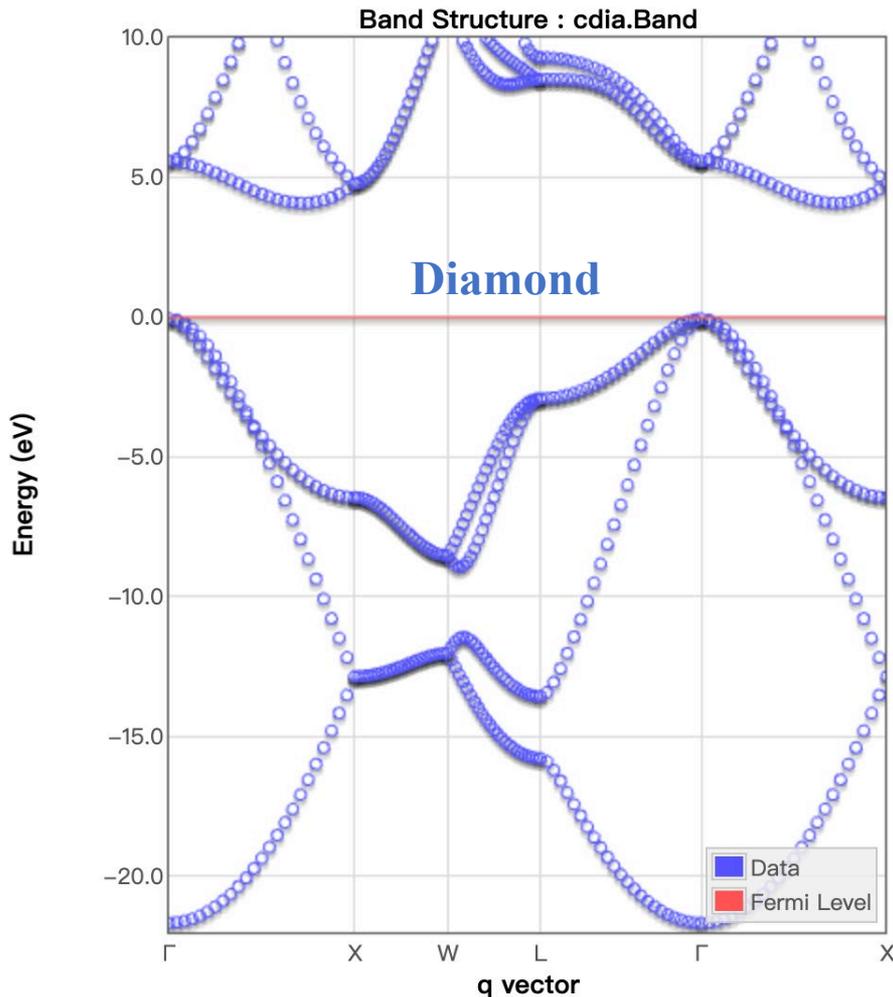
- The structure can be captured as image by pushing “Save image”, and saved as a png file. Save image
- After pushing “Save image”, and you can select a rectangular region to be saved using mouse as shown below.



- After selecting the rectangular region, the region is automatically saved as a png file of which quality can be better than that by another capture tool.

# Band Structure Viewer

- By dragging and dropping a \*.Band file onto the OpenMX Viewer webpage, one can visualize a band structure in a new tab.



- By pressing mouse left button and moving cursor up/down, the “Energy” range can be **shifted**.
- By scrolling middle wheel button, the “Energy” range can be **scaled up/down**.
- The Fermi-level line can be adjusted by controlling the “**Fermi\_Level**” slider.



# Bug report and request for development

- Any bug reports and request for development should be posted on the OpenMX Forum:

<http://www.openmx-square.org/forum/patio.cgi>

## OpenMX Forum

ENHANCED BY Google

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#### Topics



From Administrator