MONASH University
Department of Materials Science and Engineering

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Tutorial 3: Prepare Atomic Models for DFT Calculations

Background: Preparation of atomic models is the first step in DFT calculations. In this tutorial, we will start from creating primitive cell, and then apply similar methods to create supercells.

Many tools are available for preparing and visualizing atomic models. We will use VESTA in this tutorial. VESTA is a free 3D visualization program for structural models that also allows editing to some extent. It is available for Windows, MacOS and Linux operating systems.

Problem Description:

1. Create primitive cell for the following materials:

   Sodium (BCC, a=4.230 Angstrom)

   Aluminum (FCC, a=4.050 Angstrom)

   Magnesium (HCP, a=3.209 Angstrom, c=5.210 Angstrom)

   Graphene (a=2.46 Angstrom)

2. Create supercells for the following materials:

   3*3*3 Aluminum supercell

   5*3 Graphene supercell

   3*3 Bilayer graphene supercell (interlayer distance 3.35 Angstrom)

Instructions for VESTA:

1. **Initialize unit cell dimension:**

   We start by obtaining the structural data for the unit cell of the material we are interested in.

   Click "**File" -> "New Structure …**", and enter the "**New Data**" window.

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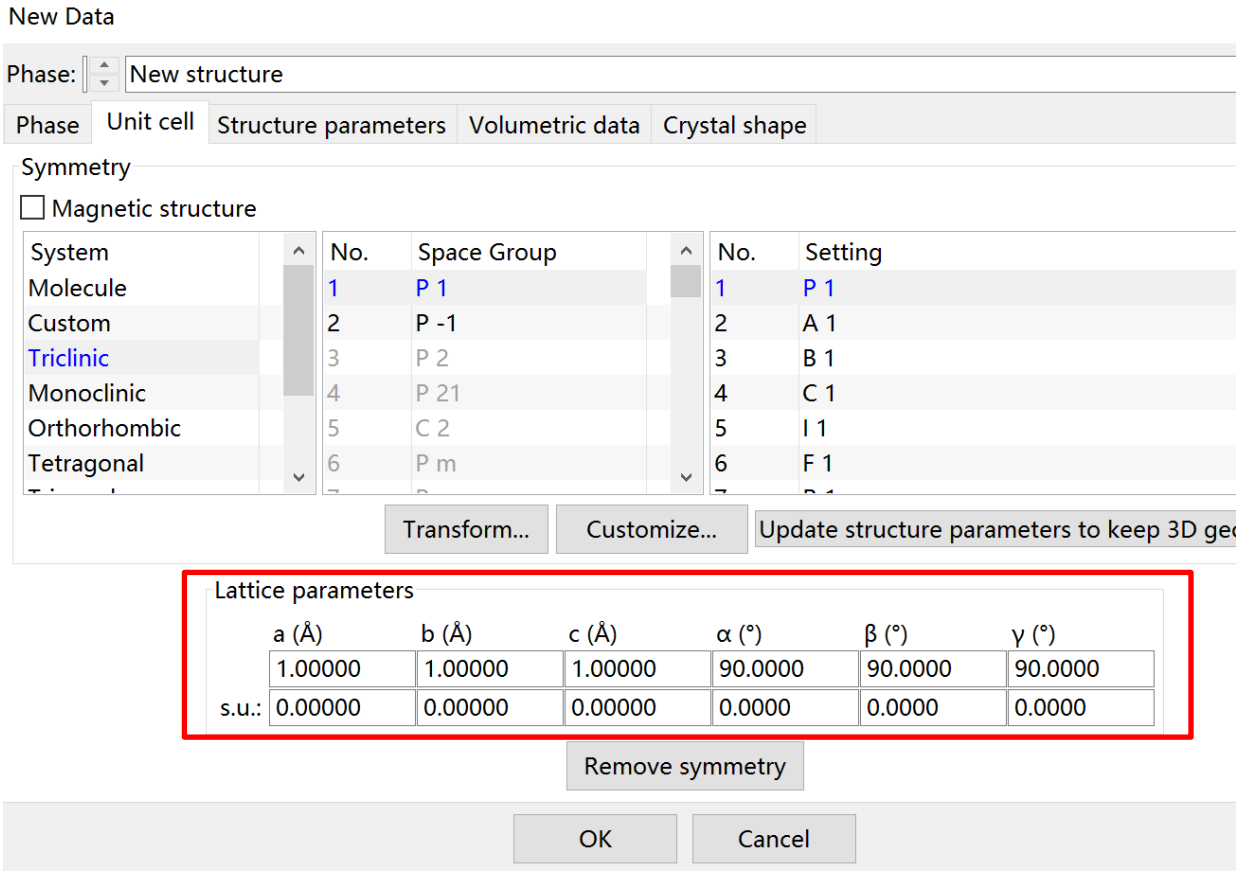
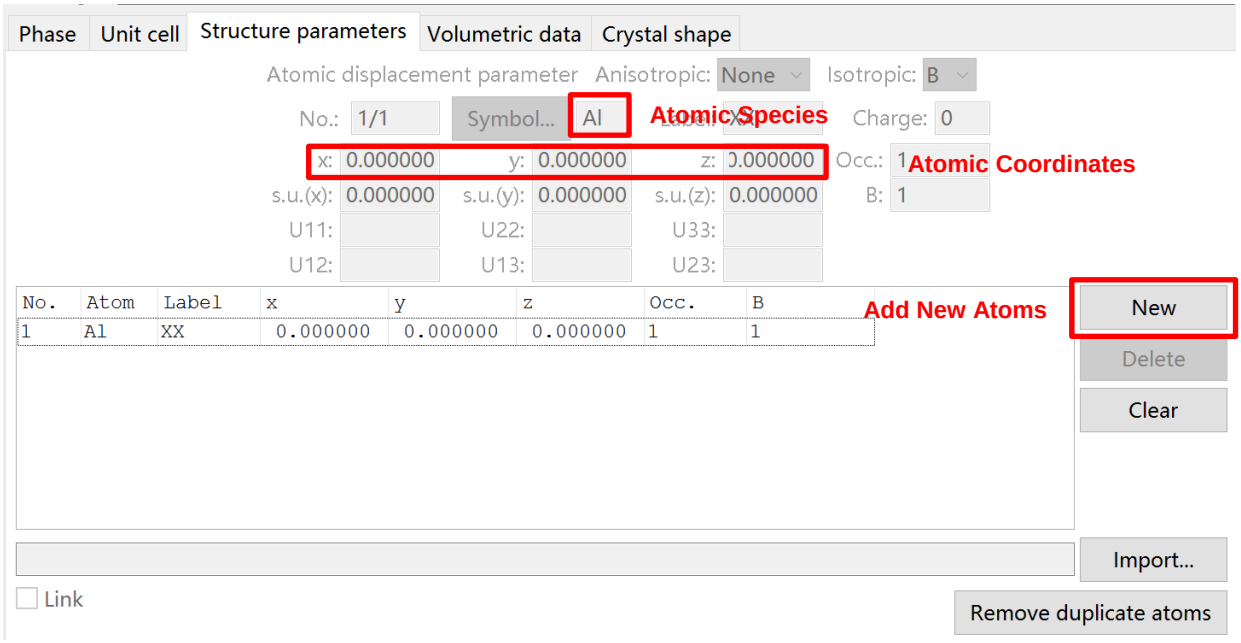


Click "**Unit cell**" tab, and enter the unit cell dimensions (highlighted in red in the figure above).

2. **Enter atomic coordinates**



Click "**Structure parameters**" tab, and fill the atomic coordinates, atomic species

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by changing the highlighted area in the figure above.

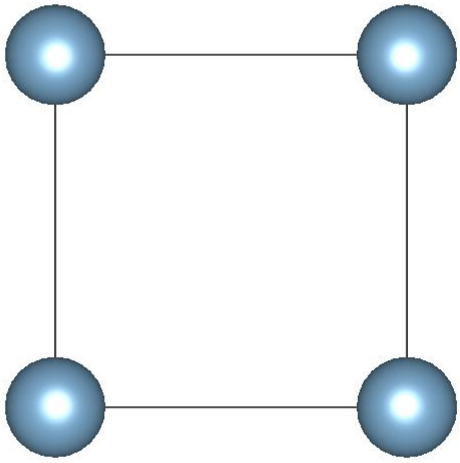
The x, y, z, coordinates are entered in fractional form. i.e. the x, y, z coordinates are entered in the form of the fraction of the cell dimension.

This means that suppose the cell lattice vectors (see “Lattice parameter” in “Unit cell” tab) are **a, b** and **c,** then any atomic coordinates are defined by:

$$x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$$

3. Visualize the structure

After Step 1 and Step 2 are completed, the atomic structure should have been visualized in the output window.



4. Make supercell

Go to **Edit -> Edit Data -> Unit cell…**

In the unit cell tab, click **Transform …,** and get make the supercell by changing the transformation matrix (highlighted in the figure below). The figure below is an example of constructing a 3*3*3 supercell.

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