

MetaChem Guide

MetaChem is to utilize augmented reality MetaGlass to build, visualize, modify and adjust molecular structures.



(The PDB code of the cover structure is 5E3M)

MetaModels Menu

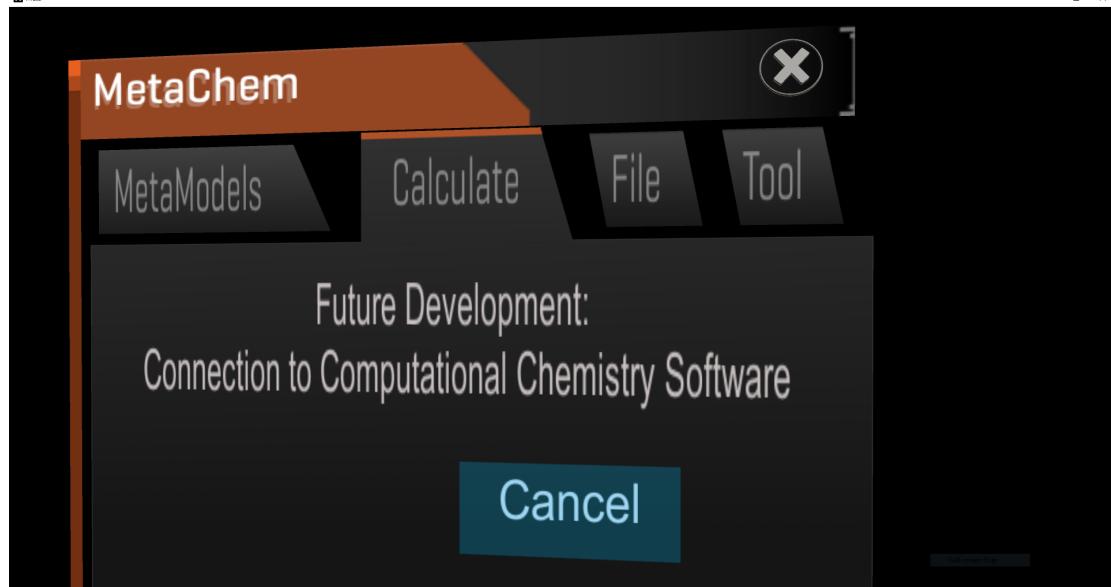
The menu panel is right in front of users, and has four sub-menus. The first one is *MetaModels*, which contains meta models for single bond and chemical elements 1-36. Clicking the thumbnail will generate a new atom or a new single bond. A convenient way to build a chemical system is to load a file (it is introduced *File* menu part).



Calculate Menu

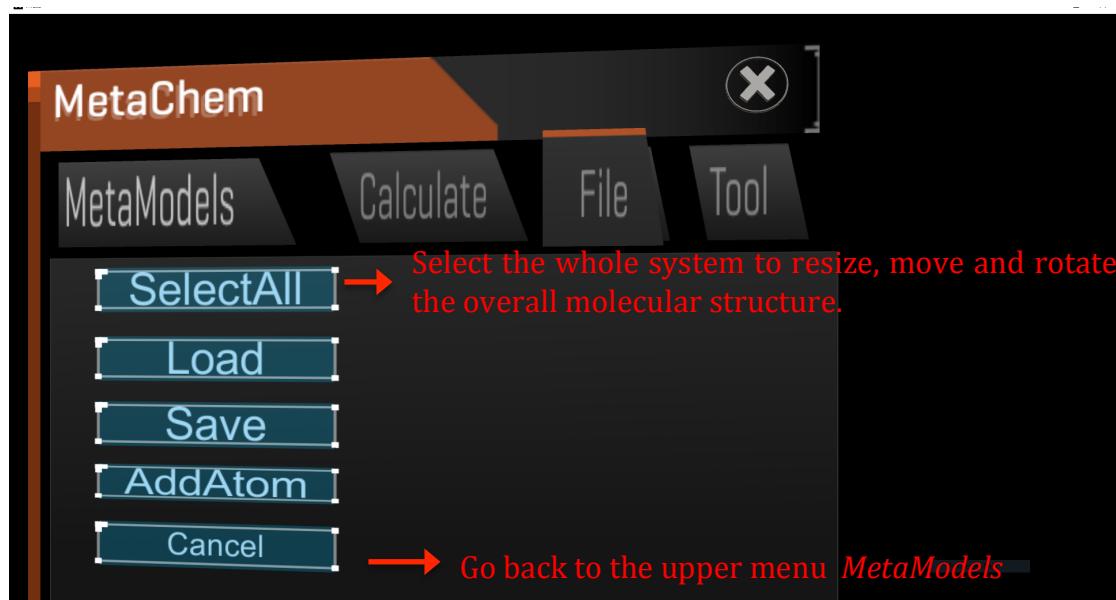
The calculation function is the main goal of MetaChem. So MetaChem can provide a 3D visualization of molecule structure and reliable chemistry and physics information of the molecule at the same time.

Click *Cancel* button to the upper menu *MetaModels*.

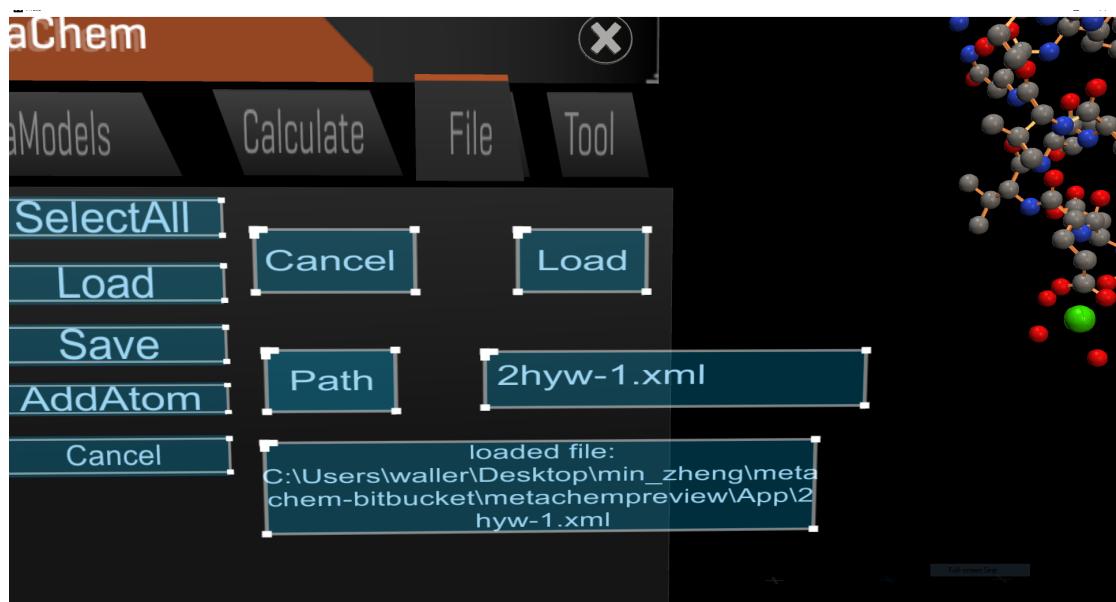


File Menu

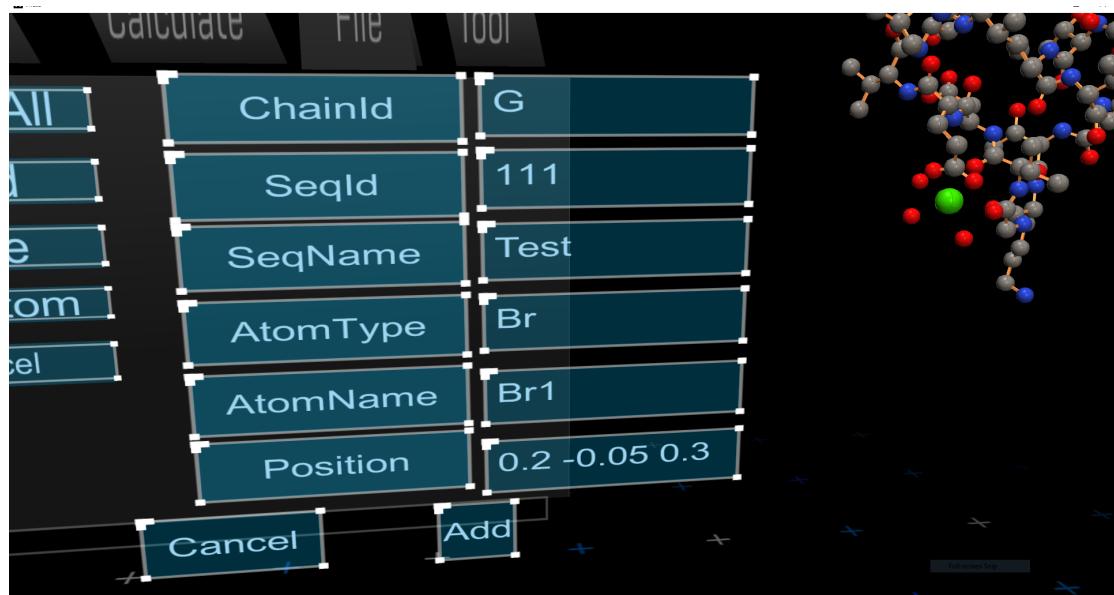
The *File* menu mainly is to load a molecule structure from a file and save a molecule structure into a file.



1). *Load* : build a molecule from a PDBML/XML file



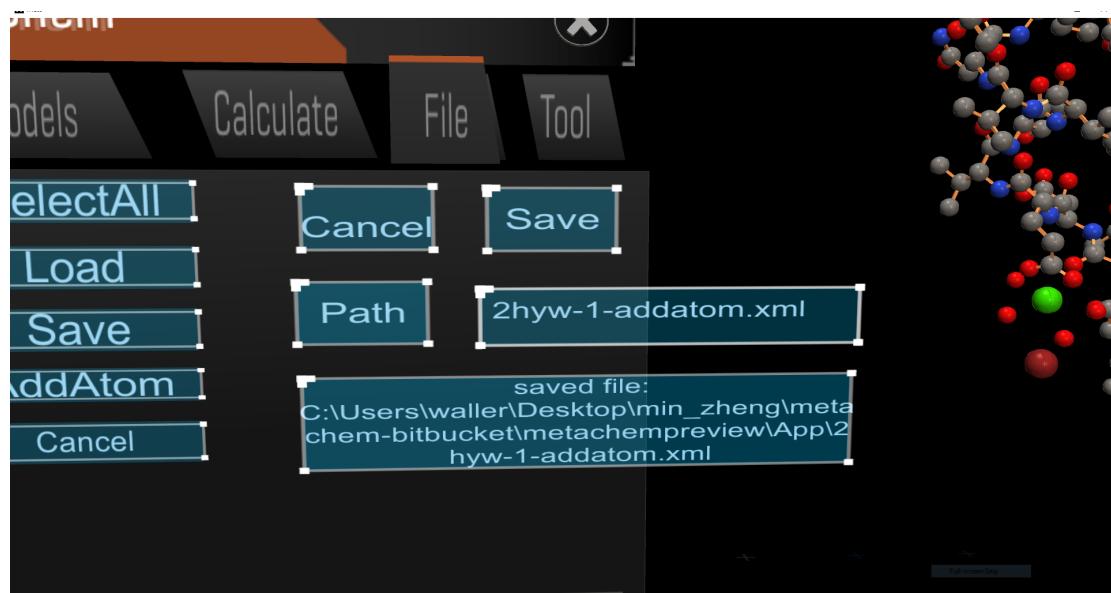
2) *AddAtom* : add a specific atom into the current molecular structure.
type the information of the new atom



then click *Add* button, we can see the new added Br atom in the following figure.



3) Save : store the current structure into a PDBML/XML file.



open the saved file 2hyw-1-addatom.xml, at the end of the file there is information for the newly added atom Br.

The screenshot shows a MonoDevelop IDE window with the XML file '2hyw-1-addatom.xml' open. The code is as follows:

```
<atom_siteCategory > atom_site
5070   <Cartn_y> -4.02800074</Cartn_y>
5071   <Cartn_z> 44.501</Cartn_z>
5072   <auth_seq_id>0</auth_seq_id>
5073   <label_alt_id>xsi:nil="true"> />
5074   <label_asym_id>Q</label_asym_id>
5075   <label_atom_id>0</label_atom_id>
5076   <label_comp_id>HOH</label_comp_id>
5077   <label_seq_id>9999</label_seq_id>
5078   <type_symbol>O</type_symbol>
5079 </atom_site>
5080 <atom_site>
5081   <Cartn_x> 28.4390068</Cartn_x>
5082   <Cartn_y> -5.718001</Cartn_y>
5083   <Cartn_z> 42.906</Cartn_z>
5084   <auth_seq_id>0</auth_seq_id>
5085   <label_alt_id>xsi:nil="true"> />
5086   <label_asym_id>Q</label_asym_id>
5087   <label_atom_id>0</label_atom_id>
5088   <label_comp_id>HOH</label_comp_id>
5089   <label_seq_id>9999</label_seq_id>
5090   <type_symbol>O</type_symbol>
5091 </atom_site>
5092 <atom_site>
5093   <Cartn_x> 20</Cartn_x>
5094   <Cartn_y> -5</Cartn_y>
5095   <Cartn_z> 30.000019</Cartn_z>
5096   <auth_seq_id>0</auth_seq_id>
5097   <label_alt_id>xsi:nil="true"> />
5098   <label_asym_id>G</label_asym_id>
5099   <label_atom_id>Br1</label_atom_id>
5100   <label_comp_id>Test</label_comp_id>
5101   <label_seq_id>111</label_seq_id>
5102   <type_symbol>Br</type_symbol>
5103 </atom_site>
5104 </atom_siteCategory>
5105 </datablock>
```

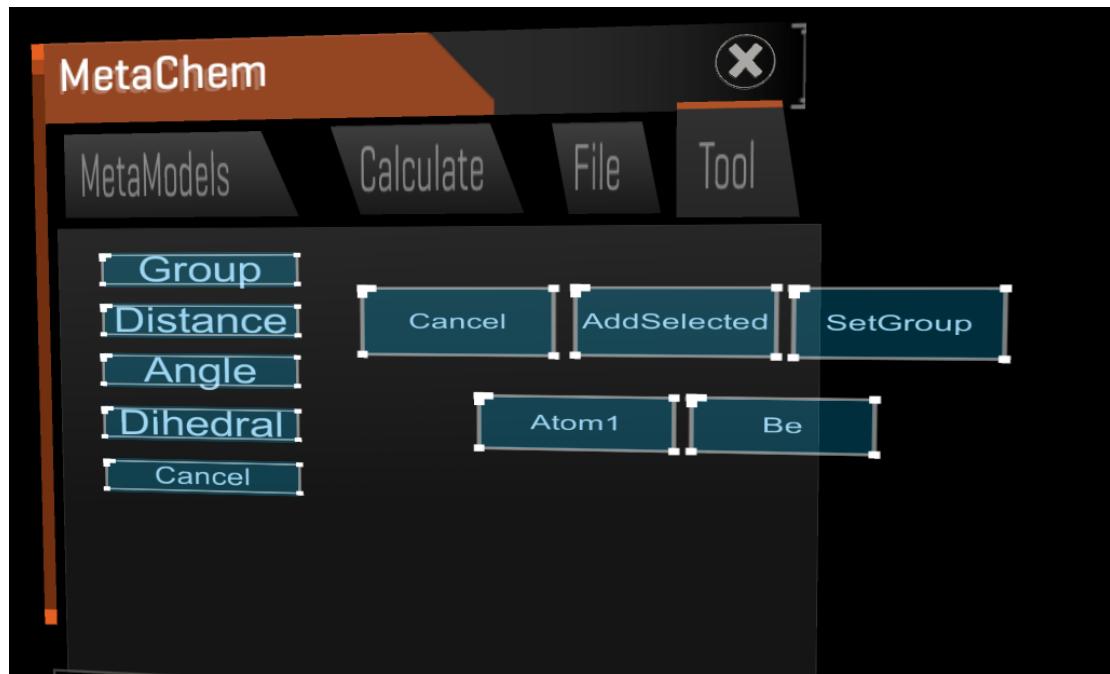
A red circle highlights the last few lines of the XML code, specifically the section defining the newly added bromine atom (lines 5092-5105).

The newly added Br atom

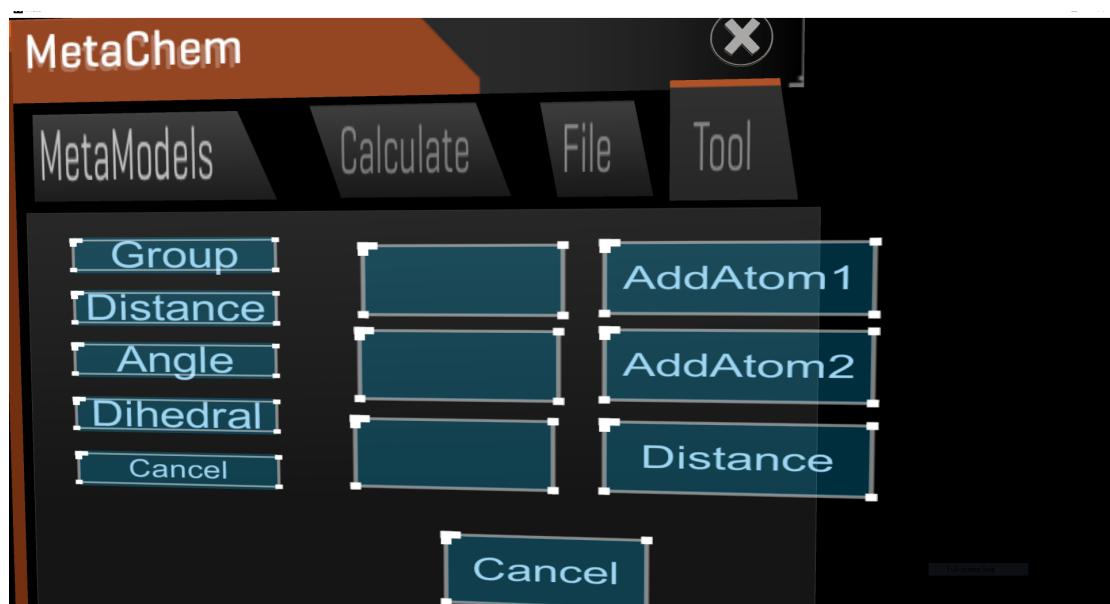
Tool Menu

The *Tool* mainly is to measure the distance, angle and dihedral.

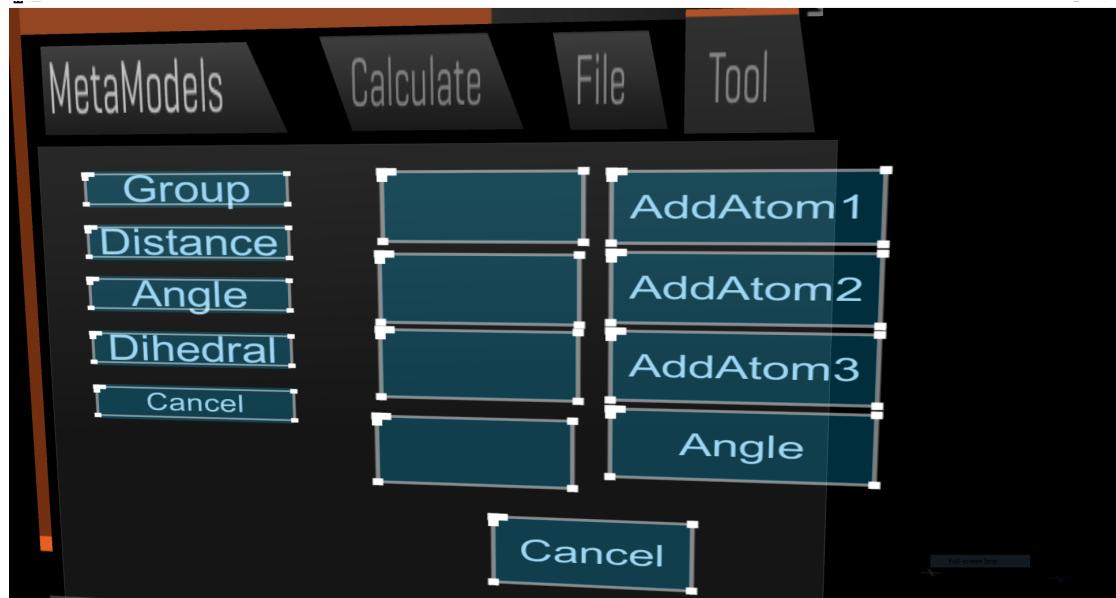
- 1) *Group*: select several objects (atoms) at the same time and operate them as one object.



- 2) *Distance*: get the distance of two atoms



3) *Angle*: get the angle of three atoms



4) *Dihedral*: get the dihedral of four atoms

