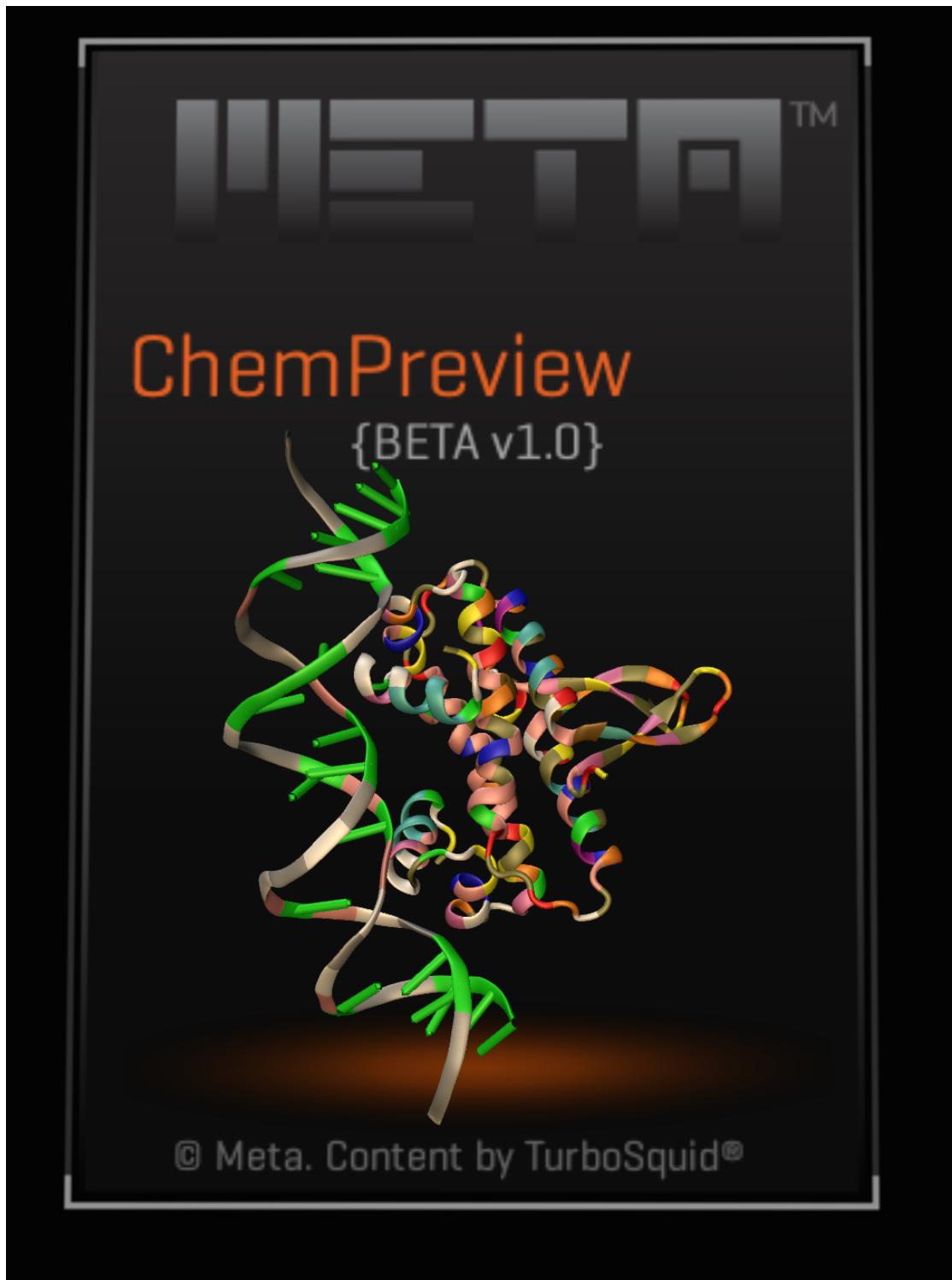


# ChemPreview Guide

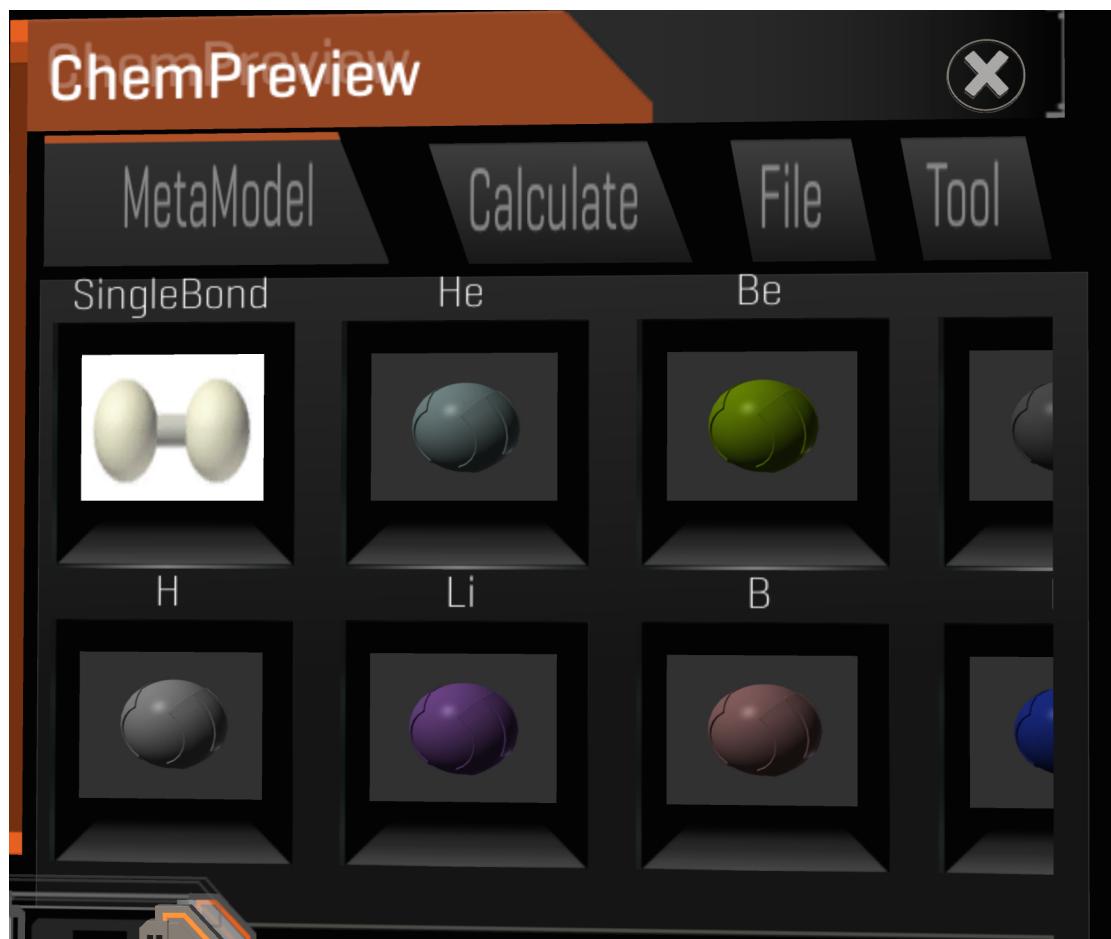
ChemPreview is to utilize augmented reality MetaGlass to build, visualize, modify and adjust molecular structures.



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

## MetaModels Menu

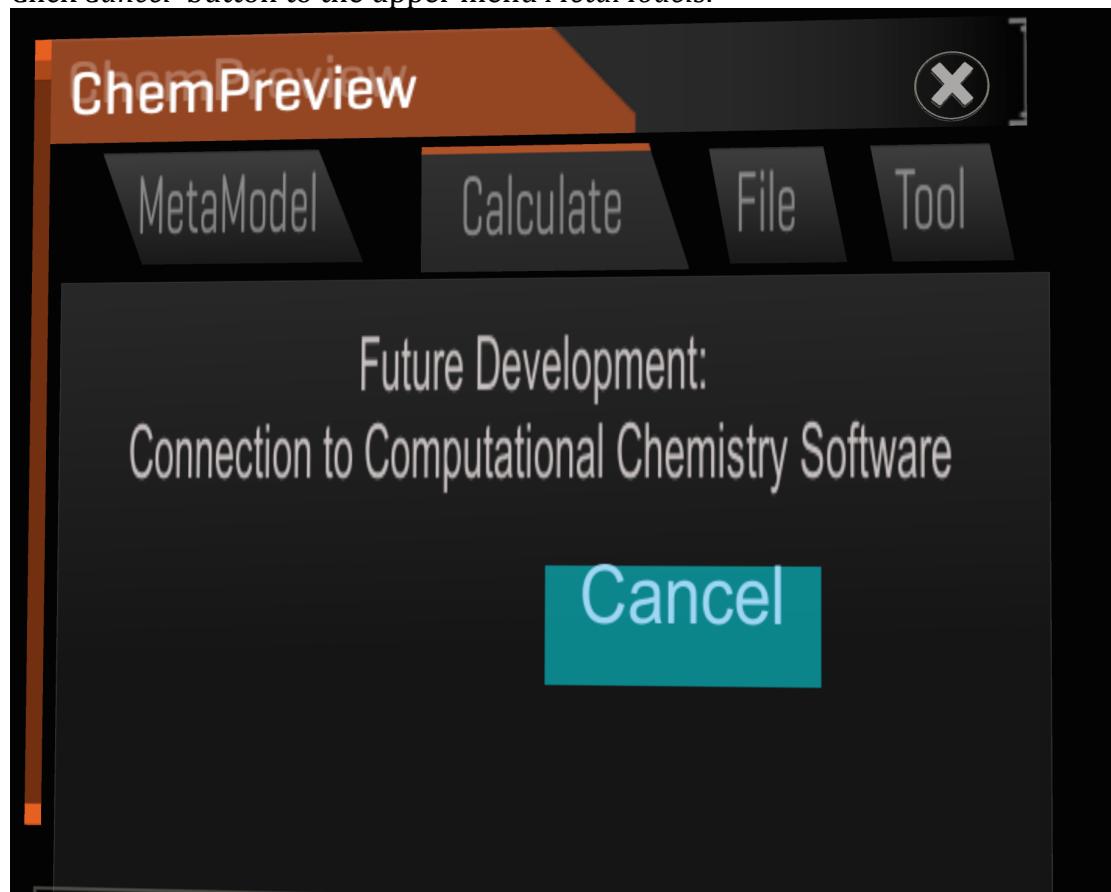
The menu panel is right in front of users, and has four sub-menus. The first one is *MetaModels*, which contains meta models for single bond and chemical elements 1-36. Clicking the thumbnail will generate a new atom or a new single bond. A convenient way to build a chemical system is to load a file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



## Calculate Menu

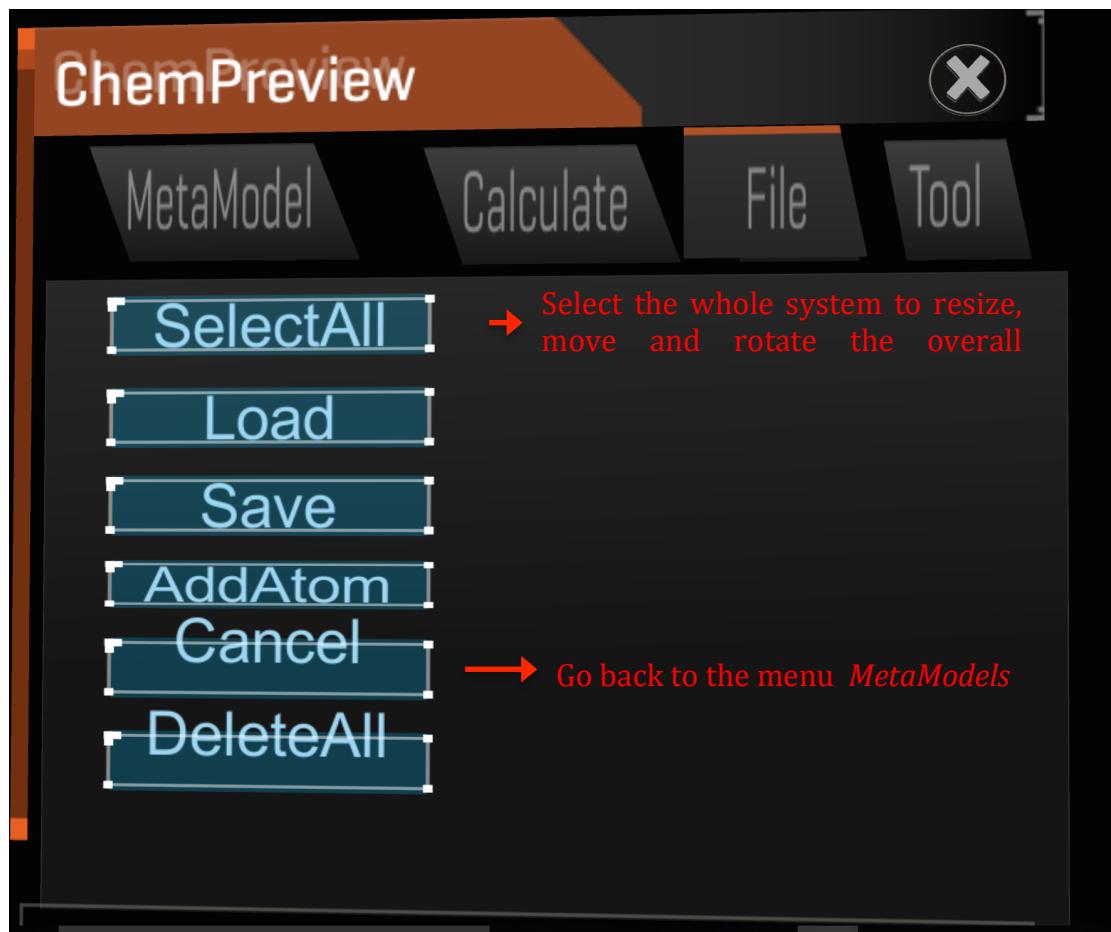
The calculation function is the main goal of ChemPreview. So ChemPreview can provide a 3D visualization of molecule structure and reliable chemistry and physics information of the molecule at the same time.

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

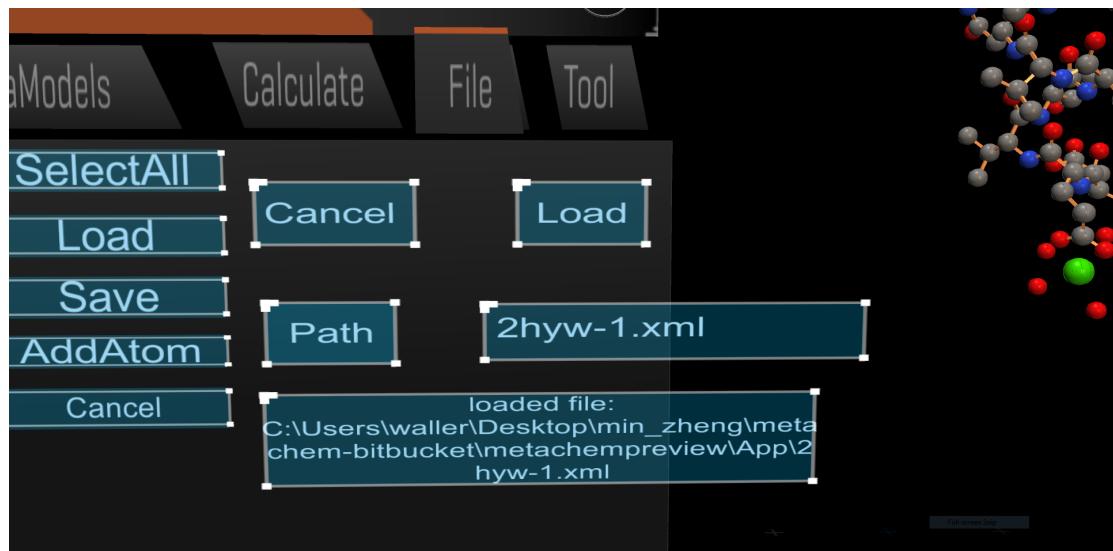


## File Menu

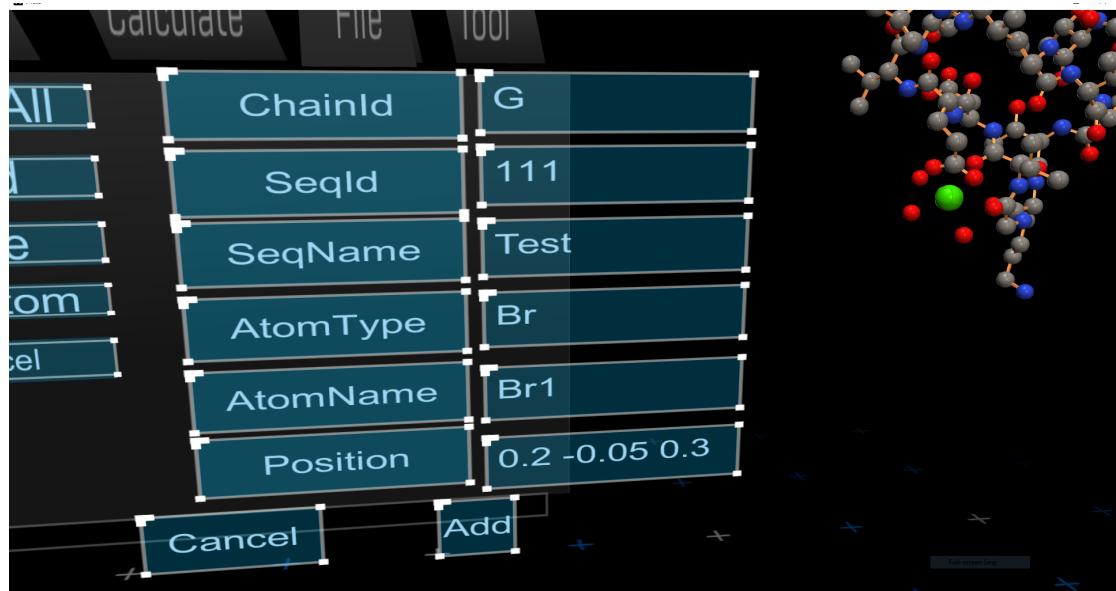
The *File* menu mainly is to load a molecule structure from a file and save a molecule structure into a file.



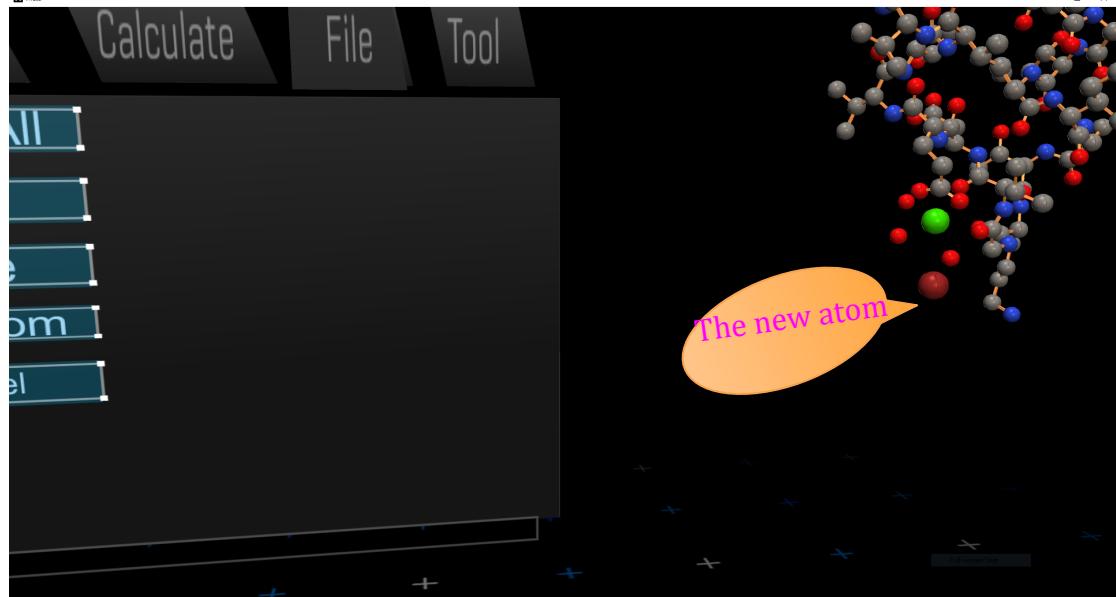
1). Load : build a molecule from a PDBML/XML file



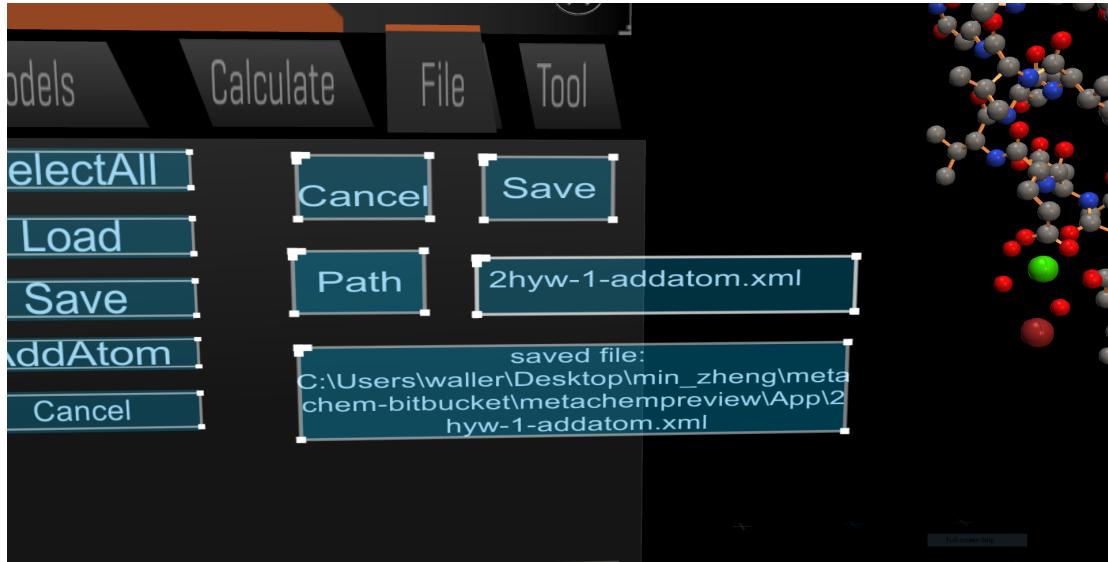
2) *AddAtom* : add a specific atom into the current molecular structure.  
type the information of the new atom



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.

```
C:\Users\waller\Desktop\min_zheng\metachem-bitbucket\metachempreview\App\2hyw-1-addatom.xml - MonoDevelop-Unity
File Edit View Search Project Build Run Version Control Tools Window Help
Debug Default Solution loaded. Press 'Control+' to search
2hyw-1-addatom.xml
<atom_siteCategory>
<atom_siteCategory id="atom_site">
<Cartn_x>-4.628000748</Cartn_x>
<Cartn_y>-4.501</Cartn_y>
<Cartn_z>44.501</Cartn_z>
<auth_seq_id>0</auth_seq_id>
<label_alt_id>xsi:nil="true"</label_alt_id>
<label_asym_id>Q</label_asym_id>
<label_atom_id>O</label_atom_id>
<label_comp_id>HOH</label_comp_id>
<label_seq_id>9999</label_seq_id>
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</atom_site>
<atom_site>
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<Cartn_z>42.906</Cartn_z>
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</atom_site>
</atom_siteCategory>

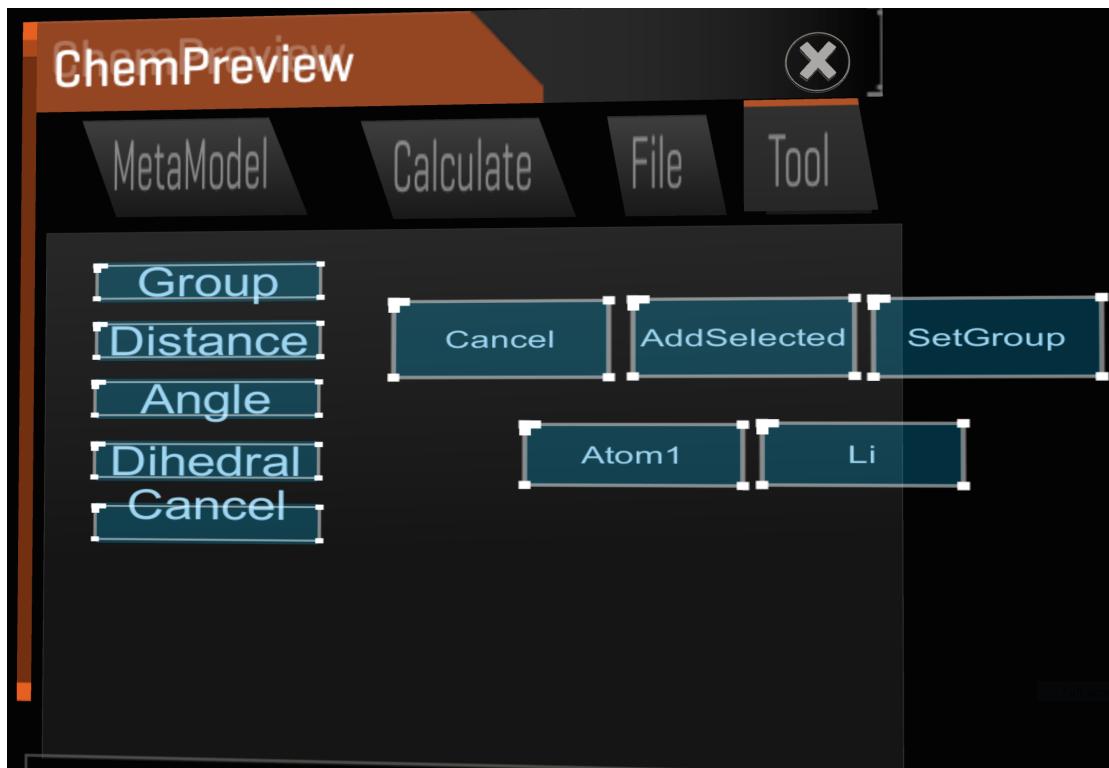
```

The newly added Br atom

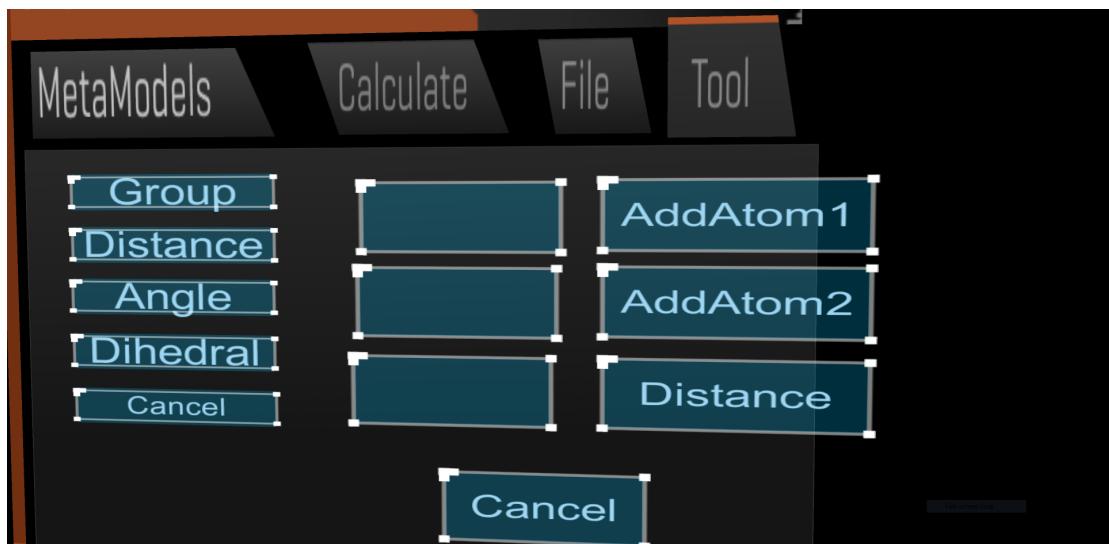
## Tool Menu

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

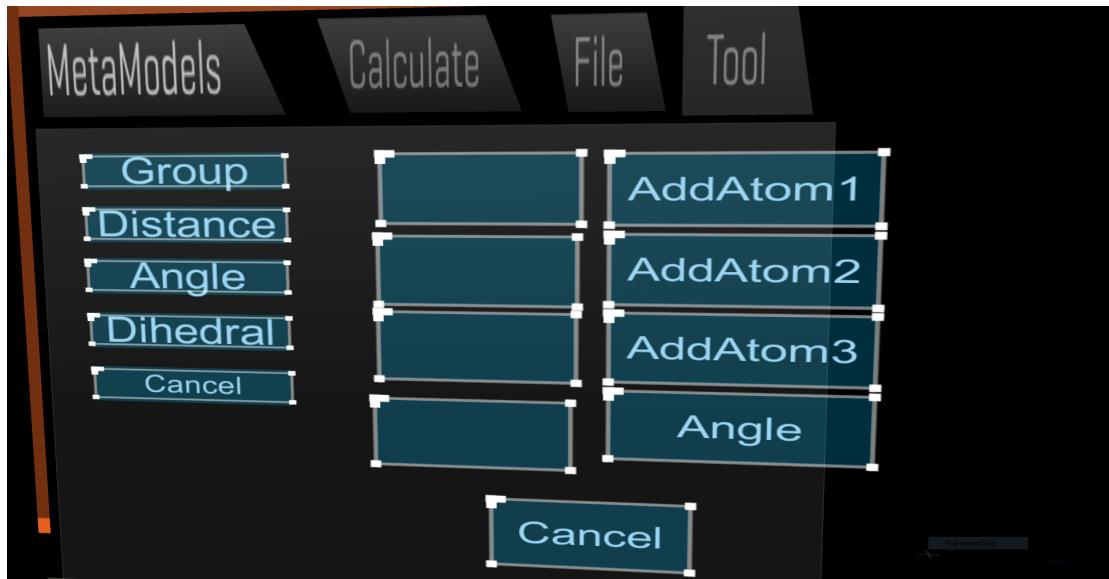
- 1) *Group*: select several objects (atoms) at the same time and operate them as one object.



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



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



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

