

MSEP.one

The Molecular Systems Engineering Platform

Feature Documentation

10/28/2024

What is MSEP.one?

MSEP.one is a free and open-source software package, developed to help with today's scientific tasks and foster designs for the future of generative nanotechnology.

The easy-to-learn interface makes building and simulating nanomachines fun and simple, perfect for students and hobbyists. Its powerful capabilities and continually expanding feature-set make it an excellent tool for professional researchers and scientists.

With its feature-rich molecular editor, MSEP.one lets users design and simulate new nanodevices. Virtual Motors provide power, while Anchors and Springs constrain their motions.

MSEP.one users will quickly and seamlessly share their inventions with an ever-growing community of molecular designers and engineers. The editor makes it easy to compose and save images of new creations.

The opportunities are limitless. The MSEP.one team looks forward to seeing what you invent!

Tutorial: What Can I Do with MSEP.one?

If you aren't a chemist or a molecular engineer then you probably want a little tutorial on how you can use MSEP.one to build your own nanomachines.

If you're already a chemist, or a molecular engineer then you probably already know what you want to build with the platform, but need to know how to implement your ideas.

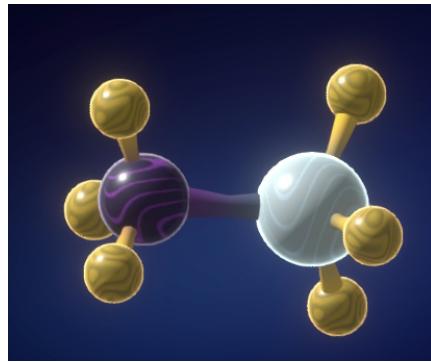
At the highest level, here are the steps you'll go through as you build your molecular machines.

1. **Create Molecules** – Build your machine parts out of bonded atoms
2. **Relax Molecules** – Relaxation causes atoms to move to positions where their forces of attraction and repulsion cancel each other out.
3. **Group Molecules** – Associate molecules so they can be moved by Virtual Motors
4. **Attach Virtual Motors to Groups** – Decide how to move your molecules
5. **Simulate Your Machine** – Run your nanomachine and see the outcome

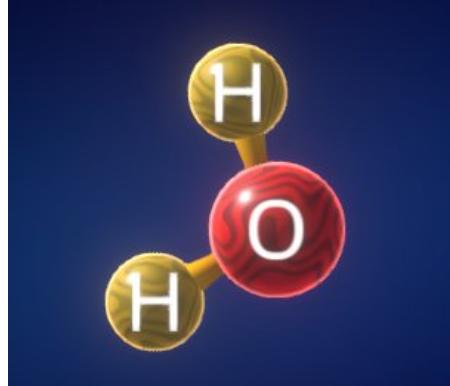
Note about relaxation: Relaxation is a basic technique, but relatively fast. For advanced simulations requiring greater accuracy, a technique called "annealing" may be used. "Annealing" is not covered by this tutorial.

- **Create Molecules**
 - You'll **create machine parts** by **connecting atoms** to each other in order to form **molecules**. There are various ways that atoms can stick together to form molecules, but in our simulation you will be connecting atoms with **covalent bonds**.
 - **What are Covalent Bonds?**
 - Covalent bonds are formed when atoms share electrons.
 - Different atoms have a different number of electrons they can share, meaning the number of bonds they can form varies.
 - For example:

- Carbon and Silicon atoms can both form up to 4 covalent bonds.



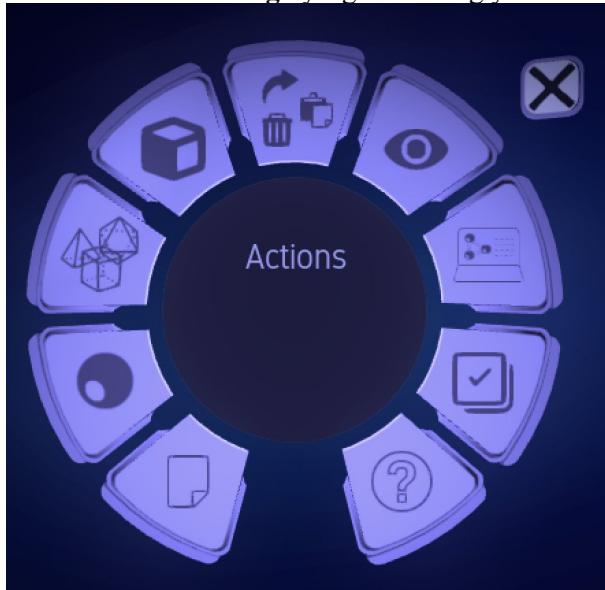
- Oxygen can form only 2 covalent bonds.



- Bonded atoms both repel and attract each other. Imagine a bond is a spring. Compress the spring and when you let it go and it will expand to its normal length. Stretch the spring and when you release it, it will snap back to its original size. The distance at which the opposing forces of a covalent bond equalizes is called the **bond length**.
- When atoms have more than one covalent bond, the angles made between these bonds are called **bond angles**.
- Due to interactions between bonded atoms, bond angle and length vary depending on a molecule's makeup.
- Even non-bonded atoms attract and repulse each other, although these forces are much weaker than bonded forces until the atoms become very close to each other. As a result, the forces between non-bonded atoms may also alter a molecule's bond lengths and bond angles.

- **Create an Atom**

- Raise the **Action Ring** by right-clicking your mouse.



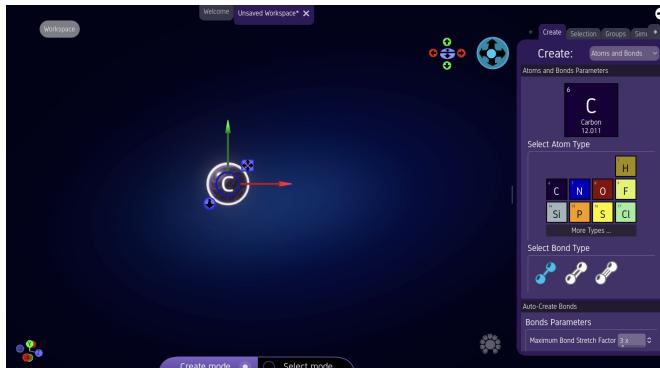
- Click on the **Atoms** button.



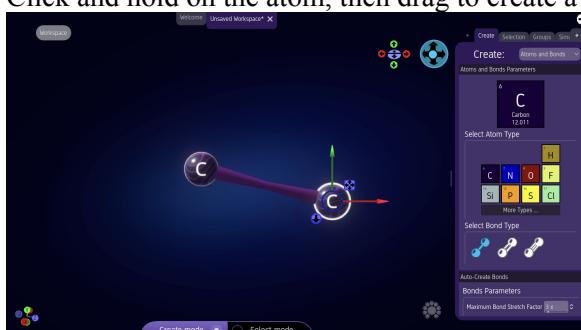
- Click on the type of atom you'd like to create.



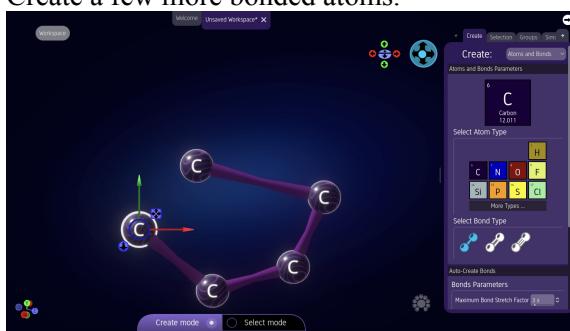
- Click in the Editor Window to create the atom.



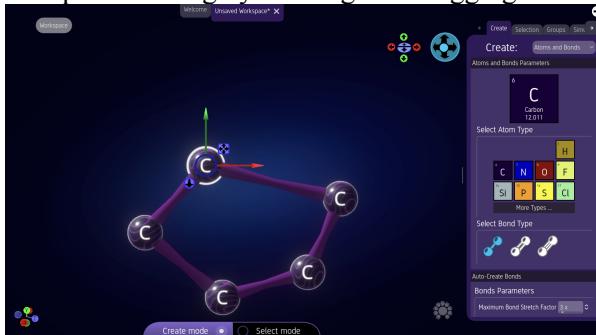
- Click and hold on the atom, then drag to create a new, bonded atom.



- Create a few more bonded atoms.



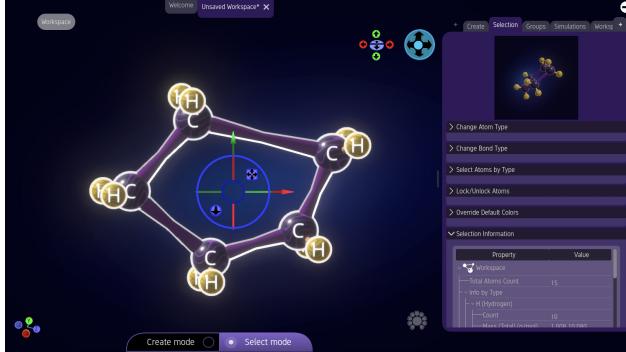
- Complete the ring by clicking and dragging a bond between the first and last atoms.



- Notice that each atom has only 2 bonds. Carbon atoms require 4 bonds. You can complete each atom's bond requirement by adding hydrogens.
- First select all the atoms and bonds by surrounding them with a selection box. Click-and-hold above and to the left of the ring, then drag until all the elements are within the selection box. Complete the selection by releasing the mouse button.



- Now, raise the Action Ring. In the “Atoms” menu, choose “Correct Hydrogens.”



- Now, each Carbon atom has its required 4 bonds.

• Relax Molecules

- Next you'll want to **Relax** your new molecule. This will adjust the bonds until each atom is at a reasonable distance and position relative to the other atoms.
- Raise the Action Ring.



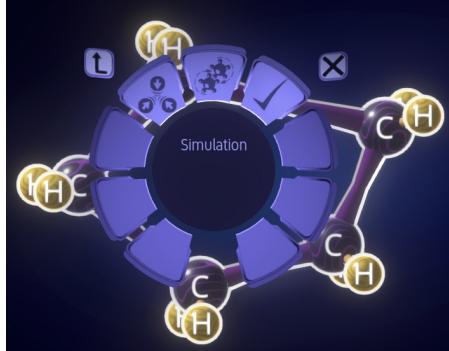
- Click the “UP” menu navigation button.



- Next, click the “Simulations” button.



- Click on the “Relax” button.



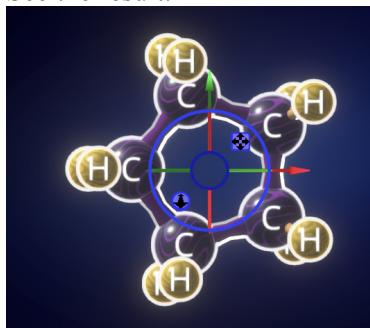
- This brings up the “Relaxation Panel.”



- In the “Relaxation Panel,” Click “Run Relaxation.”

Run Relaxation

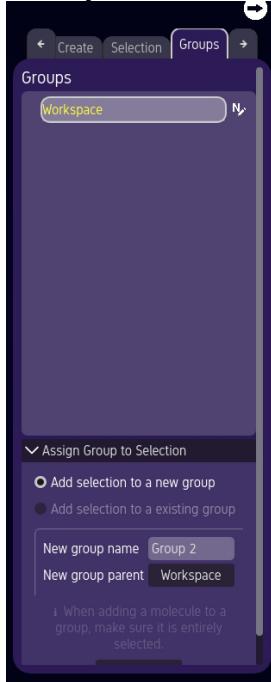
- See the result.



- **Group Molecules**

- To drive a nanomachine part with a Virtual Motor, it must be a part of a group.

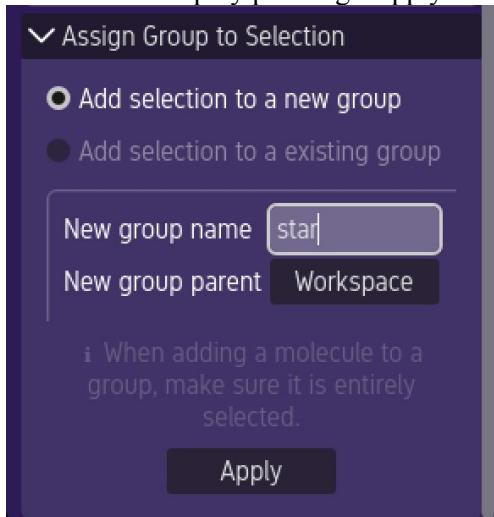
- Select your molecule, then click on the “Groups” tab in the “Features Window.”



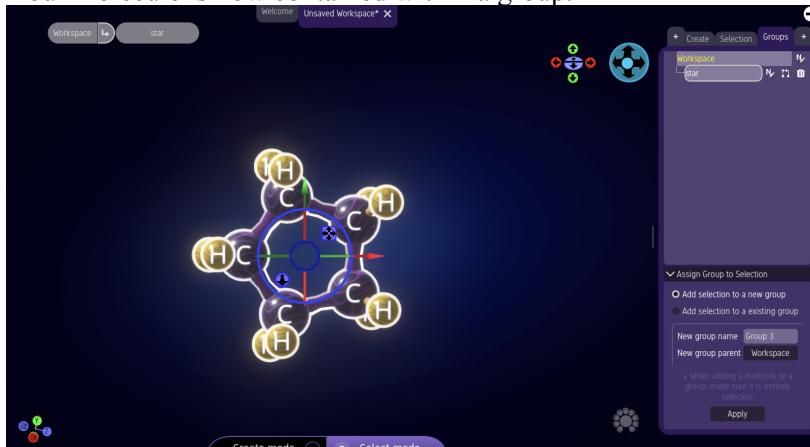
- Assign your group a name by typing it into this field.

New group name **Group 2**

- Create the Group by pressing “Apply.”

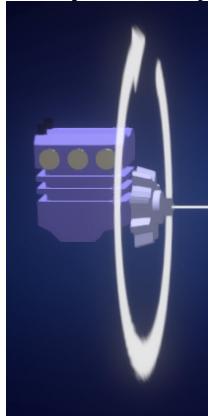


- Your molecule is now contained within a group.



- Attach Virtual Motors to Groups**

- In this example, we will use a Virtual Rotary Motor to rotate this group.
- Rotary Motors spin groups around a central axis.



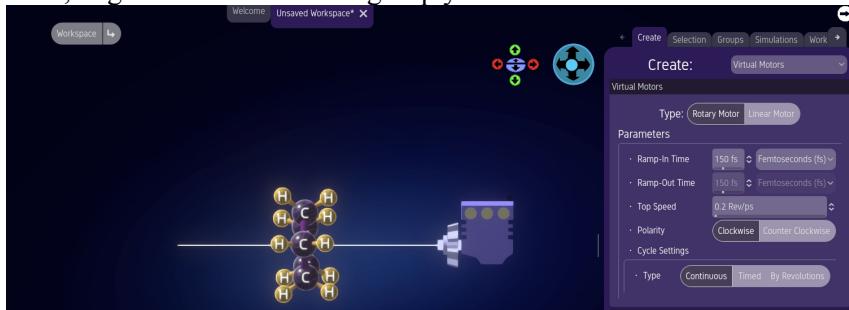
- To create a new Virtual Rotary Motor, go to the top-level of the Action Ring, then select the Virtual Objects icon.



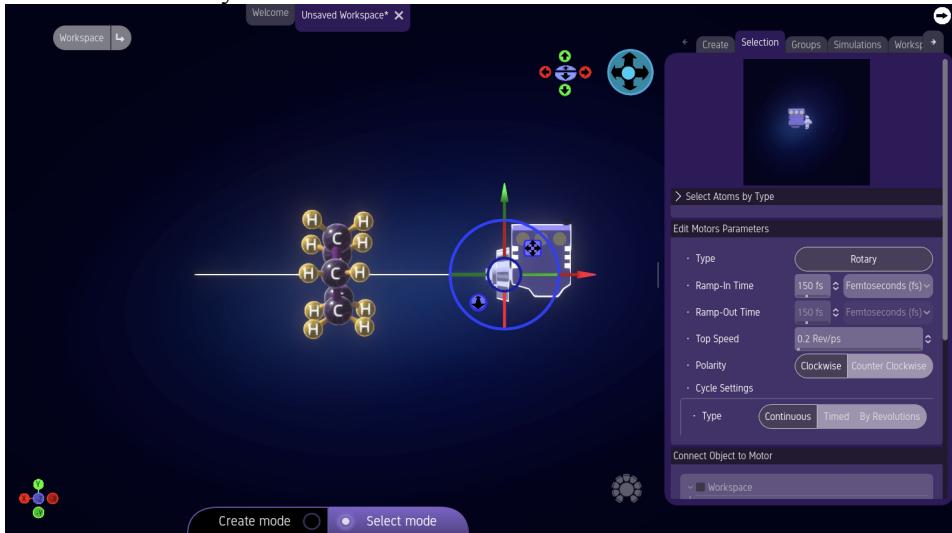
- Click on the Rotary Motor Icon.



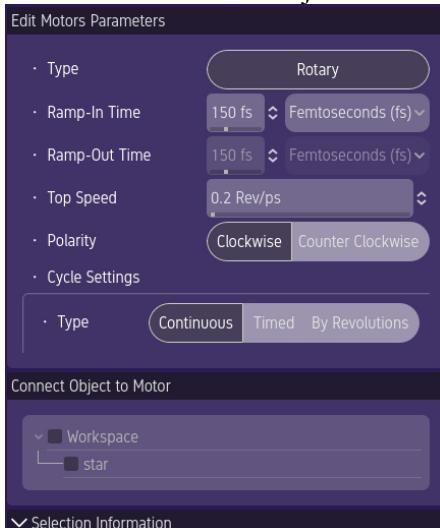
- Click in the Editor Window to create your Rotary Motor.
- In order to make simulation time something reasonable, the default rotation speed of this motor is set to an improbably fast value.
- Now, align the motor with the group you want to move.



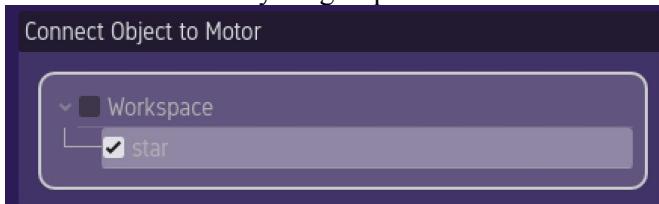
- Click on the Rotary Motor to select it.



- In the “Selection Tab” of the “Features Window” scroll down until you see your group’s name in the “Connect Object to Motor” panel..



- Click the box next to your group’s name to connect it to the motor.



- You are now ready to try out your simple nanomachine.

- **Simulate Your Machine**

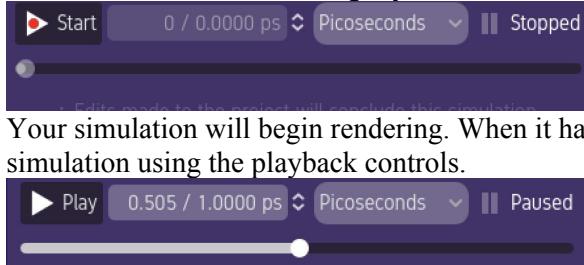
- Now that you have created a molecule, placed it in a group, and connected it to a motor, you are ready to simulate your machine.
- In the “Simulations” menu of the “Action Ring” click on the “Molecular Dynamics Simulation” button.



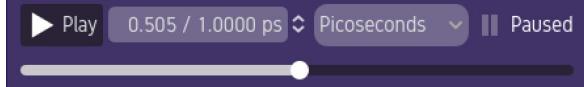
- This will bring up the “Molecular Dynamics Simulation” panel in the “Features Window.”



- Press the “Start” button to begin your simulation.



- Your simulation will begin rendering. When it has completed, you can replay the simulation using the playback controls.

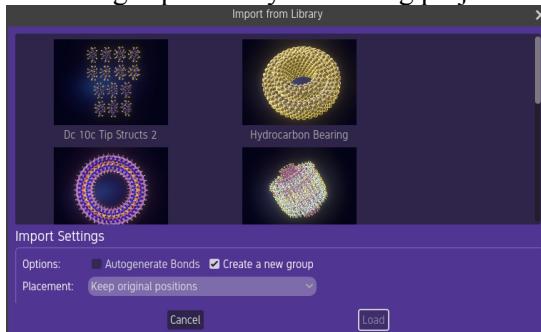


- Interlocking Gear Project Example**

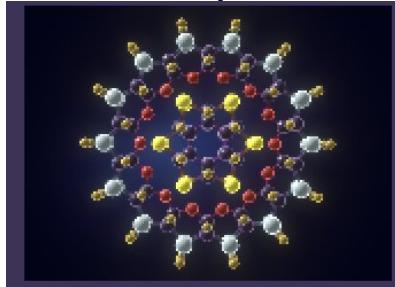
- If your simulation uses **multiple groups**, then they may interact with each other. For example, let's create a machine made up of 2 gears. A motor spins the first gear, which in turn spins a second gear.
- Start with an empty Workspace.
- In the “File Menu” of the “Action Ring” you can click on the “Import from Library” button.



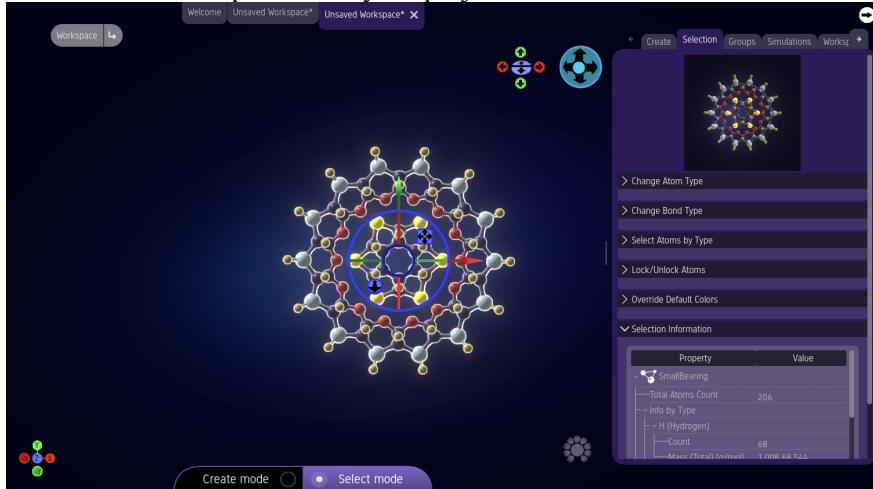
- This brings up a library of existing projects.



- Scroll down until you see the “Small Bearing.”



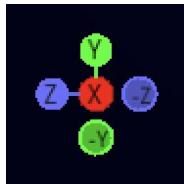
- Click “Load” to import it into your project.



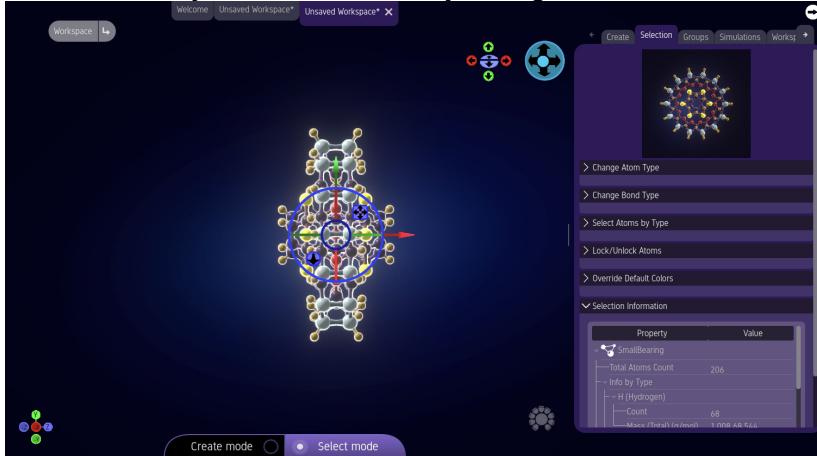
- You will see that the small bearing is already in its own group called, “SmallBearing.”

Property	Value
SmallBearing	
Total Atoms Count	206
Info by Type	
H (Hydrogen)	
Count	68

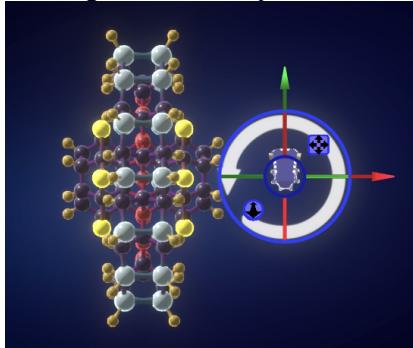
- The SmallBearing is actually made up of 2, disconnected rings. For this example, we are going to ignore the smaller, central ring.
- Click the “X Axis” button on the Editor’s Orientation Window in the lower-left of the screen.



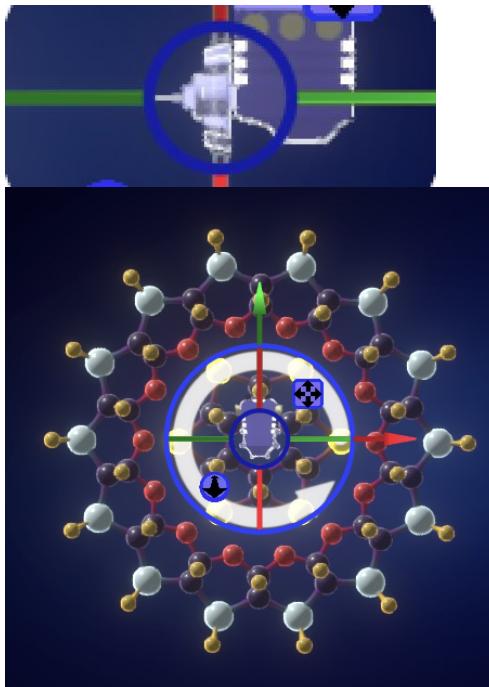
- This will rotate your camera's view by 90 degrees.



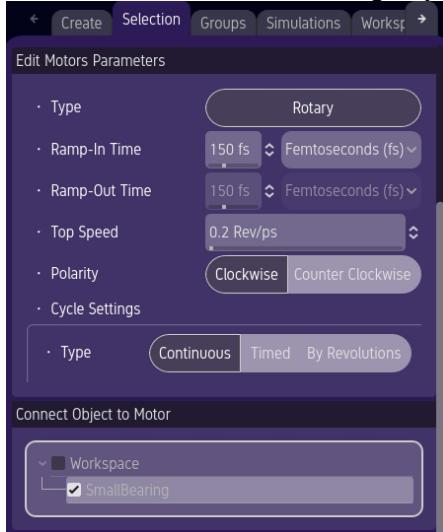
- With the group selected, create a Virtual Rotary Motor. When a group is selected, creating a motor will place it at the same depth as the selected group's center-point.



- Click and drag on the central green line of the “Transform Gizmo” to rotate the motor's direction until its drive shaft passes through the center of our “Gear.” Holding down the SHIFT key while doing this causes the rotation to jump in 15 degree increments.



- Now, connect the motor to the group.



- So far, you have been working in the “Balls-and-Sticks” view. Generally, this is easiest view for editing. Now, you will want to see your model in a representation that shows the distance at which atoms will interact with each other. For that, you will want to choose the “Mechanical Simulation” representation.
- From the top menu of the “Action Ring” choose the “View” icon.



- From within the “View” menu, click on the “Representation” icon.

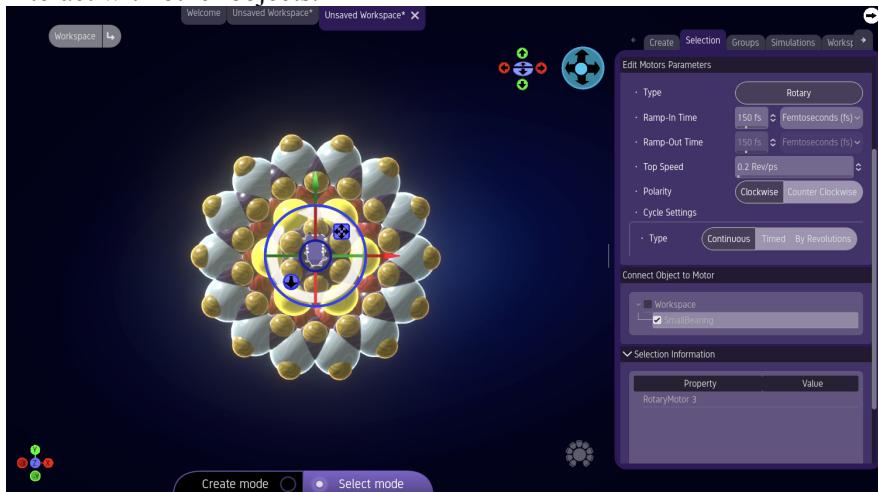


- Within the “Representation” menu, click on the “Mechanical Simulation” icon.



- Now you are viewing your project in its “Mechanical Simulation” view. In this view, the size of each atom’s spheres roughly represent the size where its electrons begin to

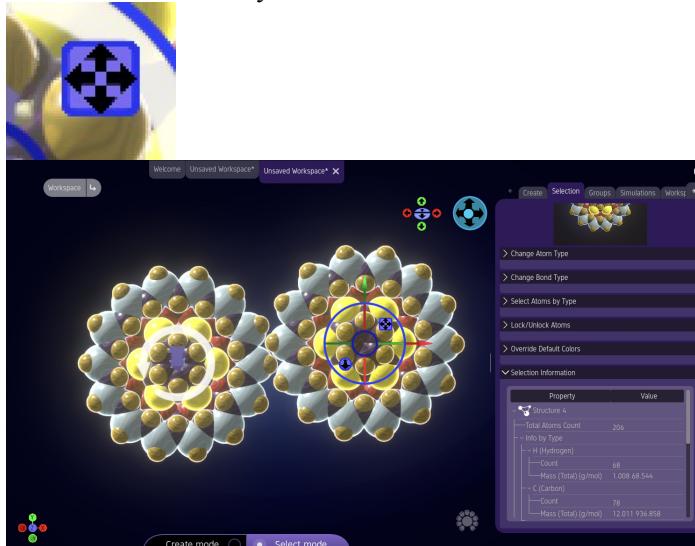
interact with other objects.



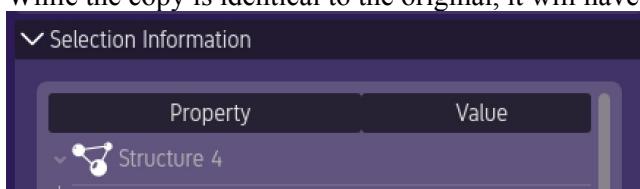
- Let's make the 2nd gear of our machine. Select the "SmallBearing" group.
- Copy and Paste the group. This can either be done from the "Edit" menu of the "Action Ring" or through the copy and paste keyboard shortcuts.



- Once you have Pasted, the copy of the bearing appears selected, but on top of the original. Click-and-drag the blue "Translation Control" of the "Transform Gizmo" to move it out of the way.



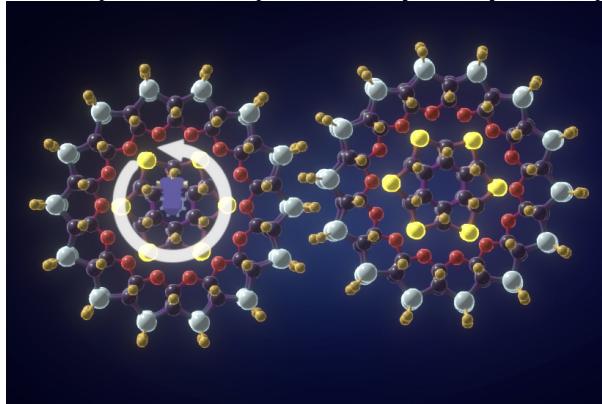
- While the copy is identical to the original, it will have a different Group Name.



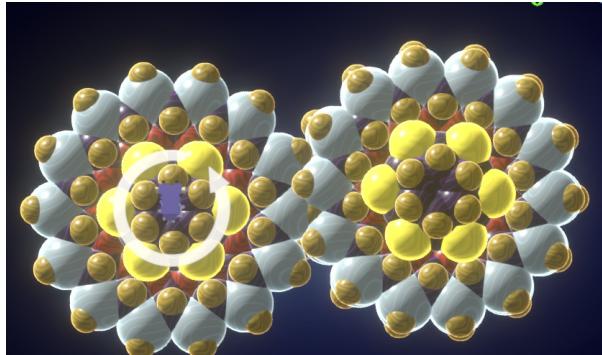
- If you have placed the copy correctly, it will look like the motor-driven first bearing will spin the second. But there is a problem. There is nothing holding the second bearing in

place. Instead of spinning, the first bearing will simply move the second bearing out of the way.

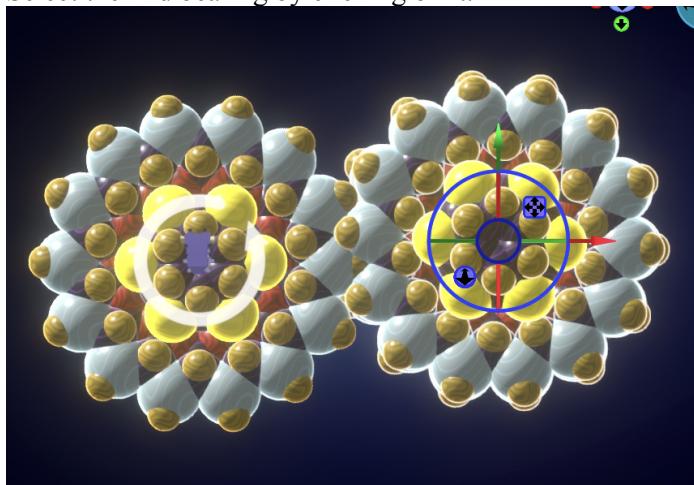
- First, make sure the 2nd bearing is meshing will with the first. Switch back to “Balls-and-Sticks” view and adjust its position.
- Don’t put atoms too close together. Make them just close enough so they can interact, but if atoms are too close, the simulation will fail. You might want to briefly switch back and forth between the “Van der Waals” and “Balls-and-Sticks” representations. If the Van der Waals spheres overlap too much, you may have a problem running your simulation.



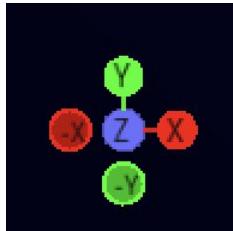
- Switch back to the “Mechanical Simulation” view.



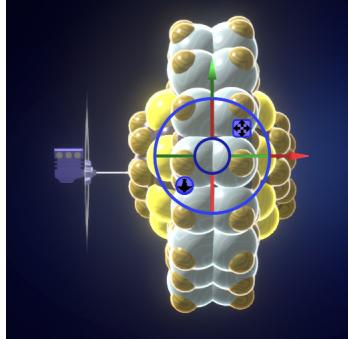
- Next, you will want to hold the 2nd bearing in position, while still allowing it to spin. For this, you can use **Springs** and **anchors**.
- **Springs** are virtual objects, representing a pulling force. **Anchors** represent an immovable point to which a **Spring** connects. The other end of a **Spring** must connect to an atom.
- We will want to create 2 anchors on either side of and aligned with the center of the 2nd bearing.
- Select the 2nd bearing by clicking on it.



- Click the red X button in the camera orientation widget in the lower left of the Editor Window.



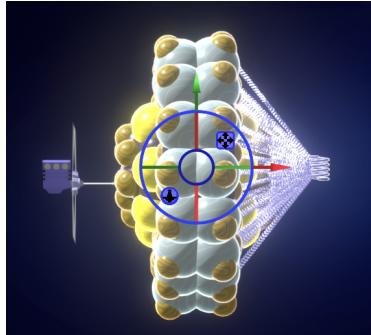
- You should now be looking at the 2nd bearing edge-on.



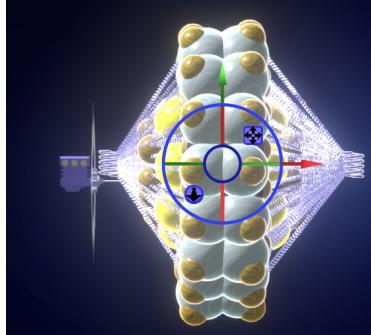
- For simplicity, we will be creating springs between our anchors and every atom in the 2nd bearing. This is not necessarily the best practice.
- From the “Virtual Objects” menu of the “Action Ring”, choose the “Anchors and Springs” icon.



- A spring will appear on your cursor.
- Hold down the **SHIFT** key and the system will draw a spring between every **selected atom** and your cursor.
- Click near the center of the 2nd bearing to create your first anchors and springs.



- Now, do the same thing on the other side of the selected bearing.



- Next, go to the “Molecular Dynamics Simulation Panel.”

- Turn off the “Relax Model Before Simulation” setting. Relaxing the model at this point may fully separate the molecules you need to interact with each other.

Relax model before running simulation
- Run your simulation.
- If you’ve done it correctly, the motor will drive the 1st bearing, which will in turn, drive the second.
- **Play with Your Own Creations**
 - MSEP.one has many, many more features and settings to play with. Now that you have the basics down, try creating your own inventions.
 - As you work on your own projects, MSEP.one will probably provide feedback in the form of Warnings and Alerts. Don’t let these stress you out. If you’re new to MSEP.one don’t feel like you have to address them all. They are there to further your understanding of molecular engineering.
 - Have fun!

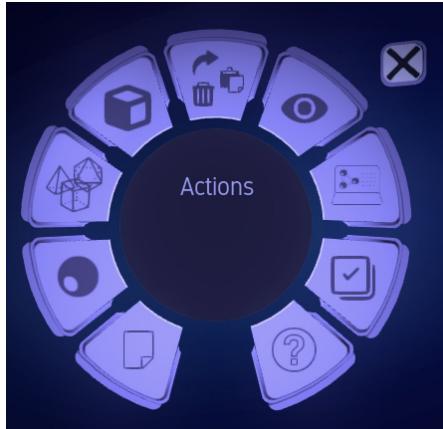
What are MSEP.one’s Features?

- Create, bond, and position Atoms
- Create 3D Reference Shapes on which Atoms can be placed
- Save and Load MSEP.one projects
- Import PDB files
- Run Relaxation, Molecular Dynamics, and Model Validation simulations
- Create Small Molecule Fragments from a robust library
- Create Object Groups
- Drive molecule movement through Linear and Rotary Virtual Motors
- Validate models for scientific accuracy
- Capture and Save project images
- Auto-Bond Adjacent Atoms
- Correct the number of Bonded Hydrogen Atoms in a Molecule
- Sample Project Library
- Visually represent Atoms and Bonds as Ball-and-Stick, Van der Waals, Mechanical Simulation, Sticks, Enhanced Sticks, Enhanced Ball-and-Stick
- Customize Atom Colors
- Customize Project Workspace
- Intuitive “Action Ring” Interface
- Feature Search Box
- Measurement Tool
- Editing Suite: Cut, Copy, Paste, Delete, Undo/Redo, Select, Grow/Shrink Selection, Select By Atom Type, etc.

MSEP.one How-To:

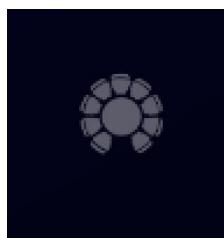
1. Action Ring

- a. The Action Ring helps you quickly find the program's most-used functions.



- b. To raise the Action Ring:

- i. Press the <TAB> key
- ii. Click the right Mouse Button
- iii. Click on the Action Ring Icon in the lower-right of the MSEP.one Editor Window.



- c. To hide the action ring:

- i. Press the <TAB> key
- ii. Click the right Mouse Button
- iii. Click on the Action Ring Icon in the lower-right of the MSEP.one Editor Window
- ii. Click the “Close Action Ring Button”



- d. The Action Ring is full of icons. When you roll over an icon with your mouse, the Action Ring displays the icon's function.

- e. An Action Ring icon can represent an organizing folder or an MSEP.one feature.

- i. For example, at the top level of the Action Ring, if the user clicks the “Atoms” icon, the ring will display the “Atoms” sub-folder. Here, you’ll find all of the

MSEP.one features related to the creation of Atoms and Bonds.



- f. To move up one Action Ring level, press the “Up Menu” button.

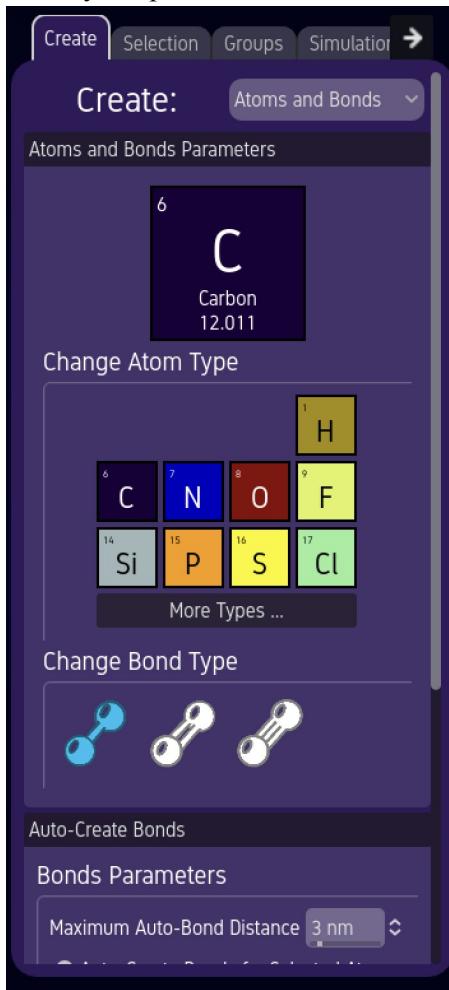


- g. Some Action Ring menus have more options than can be displayed at one time. Use the arrow keys at the bottom of the Action Ring to page through a menu’s options.



2. Feature Window

- a. When you open MSE.P.one, the “Feature Window” appears at the right of the screen.

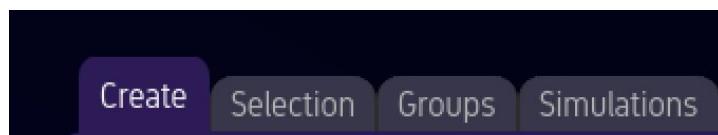


- b. You can collapse and expand the Feature Window by using the arrow button at its top right.

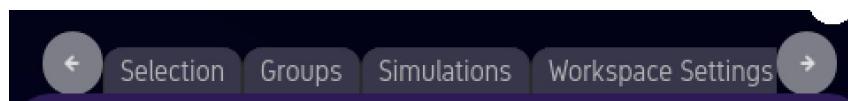


- c. To resize the Feature Window, click-and-hold then grab the Resize handle at the center-left.
d. To manually select one of the Feature Window’s various screens:

- i. Click on one of the Feature Window’s “tabs.”



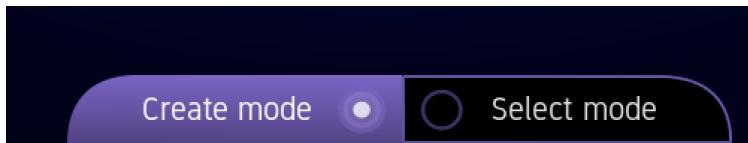
- ii. Cycle through the Feature Window’s screens with the gray arrow buttons at each end of the tab bar.



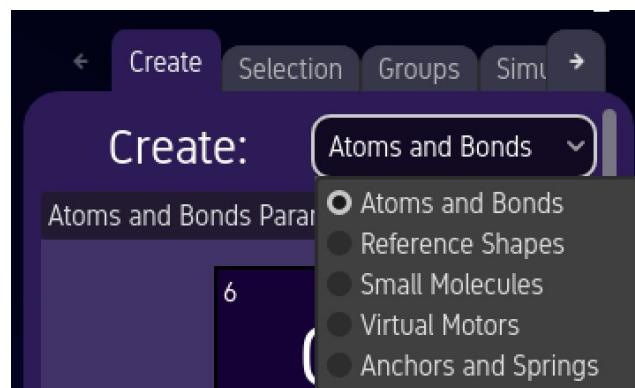
3. Creating Atoms and Bonds

- a. To create an Atom (or any other object appearing in the Editor window) you must be in “**Create Mode**.” “Create Mode” defaults to off, but switches on automatically when you choose an option from the Create Menu. You can manually toggle between “Create

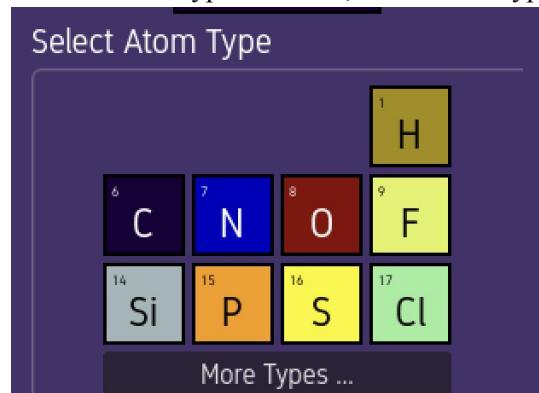
Mode” and “Select Mode” with the buttons at the bottom of the editor window.



- i. From the Action Ring
 1. Raise the Action Ring.
 2. Click on the Atoms icon.
 3. From the Atoms menu, click an icon to select the type of Atom you'd like to create.
 4. The Ring Menu will disappear, and the Feature Window will switch to the Create->Atom panel with the chosen atom type already selected.
 5. When you click in the Editor window, a new atom is created.
- ii. From the Feature Window
 1. Click on the “Create Tab” at the top of the Feature Window.
 2. Make sure “Create Atoms” is selected from the Create pull-down menu:



3. In the “Atom Type” chooser, click on the type of atoms desired.



4. Click in the Editor Window to place an Atom of the selected type.
- iii. From the “Interactive Table of Elements”
 1. Press the “More Types” button at the bottom of the “Atom Type” Chooser in the Feature Window. This will bring up the “Interactive Table

of Elements.”

The image shows a standard periodic table of elements with a search bar at the bottom labeled "Search element". The search bar contains the letter "I" and has a magnifying glass icon.

2. To choose an Atom Type, click on one of the table's colored squares. If MSEP.one does not support an Atom Type, its box will be grayed out and not selectable.
3. To locate a specific Atom Type in the Interactive Table of Elements, type the name of the desired element in the search bar.

The image shows the same periodic table as above, but the search bar at the bottom now contains the word "Potassium". The search bar has a magnifying glass icon.

b. Creating Bonds

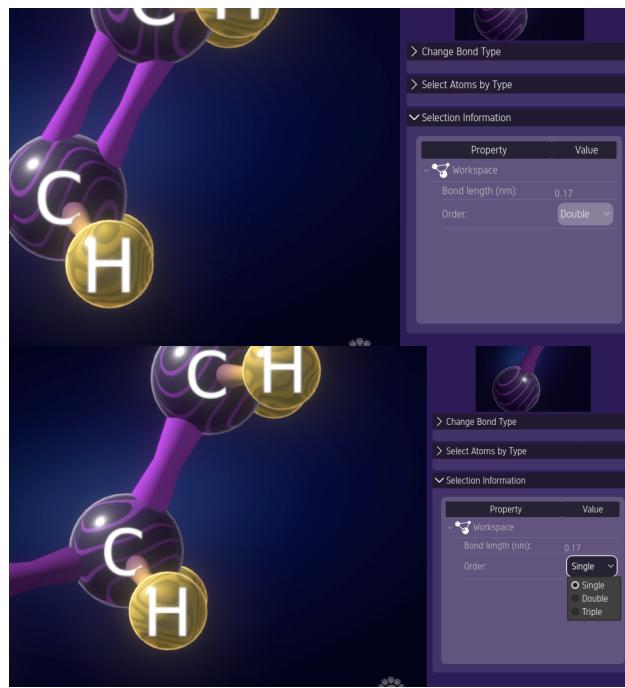
- i. First, from the Create->Atoms and Bonds panel, select the desired bond type by clicking on its corresponding bond icon. The icons represent Single, Double, and Triple Bonds.

Change Bond Type

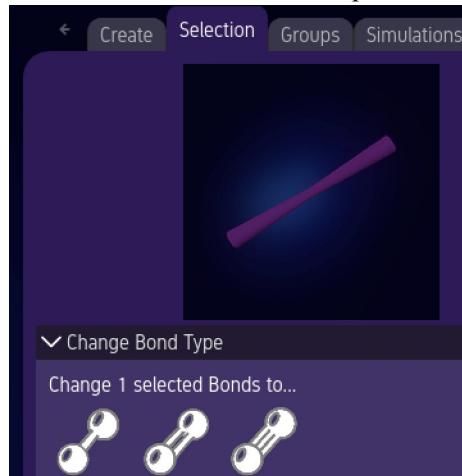


ii. Changing Bond Types

1. To change the Bond Type of an existing bond, select it. Look for the Selection Information panel of the Selection Tab. Then change the bond's type by changing its Order from the Order pull-down list.



2. Another way to change bond types is to select the bonds you want to change, then expand the “Change Bond Type” panel in the Selection Tab. Click on the icon that represents the bond type you desire.



iii. Create a Chain of Bonds

1. While holding down the <SHIFT> key, click in the Editor Window. Each click will create a new atom, bonded to the previous.

iv. Connect Existing Atoms

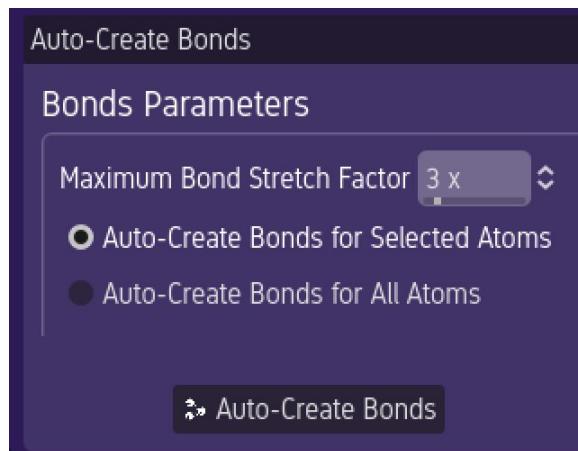
1. Click and hold on the first atom, then drag a bond until the cursor is over the target atom. Release the mouse button to create the bond.

v. Auto-Create Bonds

1. This feature will automatically bond atoms within a maximum bond distance.
2. From the Ring Menu, click on Atoms, then select the “Auto-Create Bonds” icon.



- This will bring up the Create->Atoms and Bonds panel in the Feature Window.



- This feature will only bond atoms whose distance is equal to or less than the value entered in the “Maximum Auto-Bond Distance” parameter field multiplied by the maximum bond length between the two atoms.
- When ready, press the “Auto-Create Bond” button to instantiate the bonds.

vi. Attaching Atoms to Shapes

- Reference shapes serve as forms to help users make interesting molecules.
- You can apply atoms to the surfaces of shapes by:
 - Select an atom type
 - Move the cursor over the desired shape
 - Turn on the “Snap to Reference Shape surface” toggle in the Create Panel.

Snap to Reference Shape surfaces

- Click to place atom
- c. Correct Hydrogens
- After creating a molecule (or molecules), you can ensure that it has the correct number of bonded hydrogen atoms by using the “Correct Hydrogens” function.
 - To Correct Hydrogens:

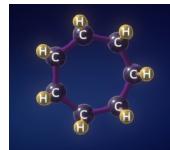
- Select the atoms and molecules you want to correct.



- From the Action Ring, go to the Atoms submenu and select the “Correct Hydrogens” icon.



- This will add a Hydrogen atom wherever an atom lacks the correct number of bonds.

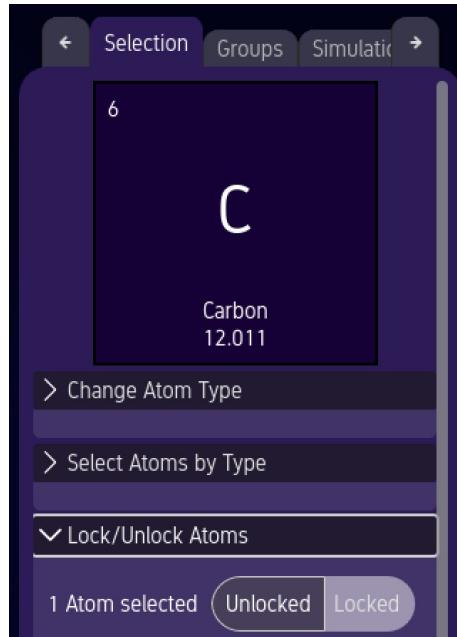


- You can also correct hydrogens for selected atoms by:
 - For Mac - press <SHIFT> + <COMMAND> + H
 - For Windows and Linux – press Ctrl+Shift+H

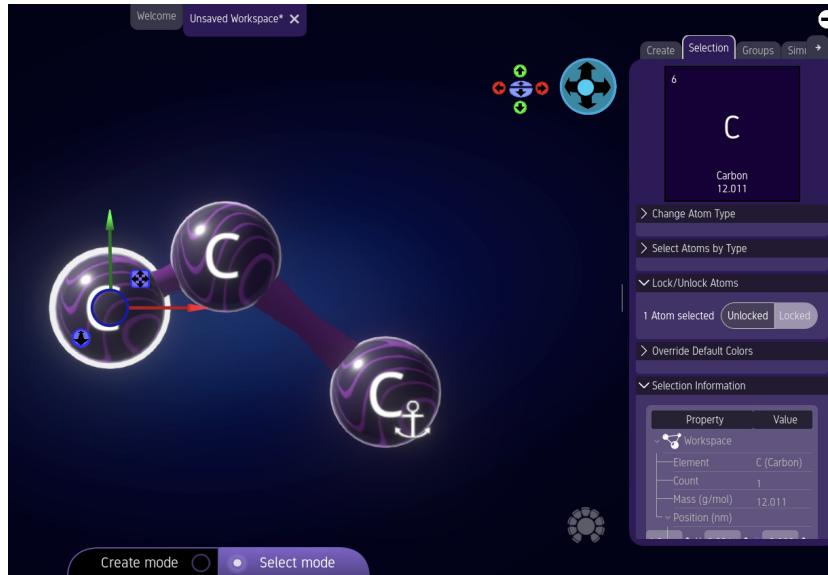
iii. Lock / Unlock Atoms



- When an atom is locked, it will not move during simulations. For example, if you are relaxing a molecule and one of that molecule’s atoms is locked, the locked atom will stay put during the relaxation.
- When an atom or atoms are selected, the Lock / Unlock Atoms panel will appear in the Feature Window’s Selection Tab.



- When “Show Atom Labels” is enabled, an Anchor Icon appears on Locked Atoms.

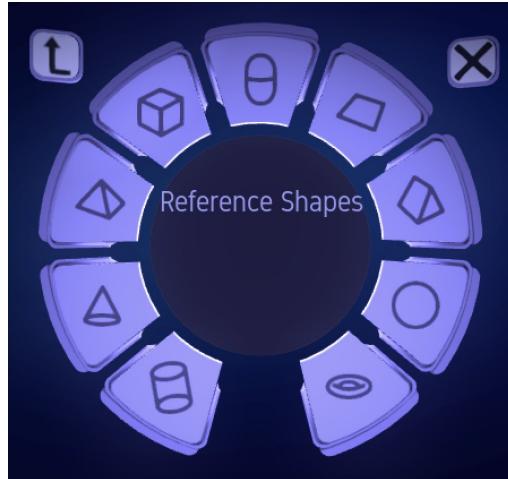


- Creating Reference Shapes

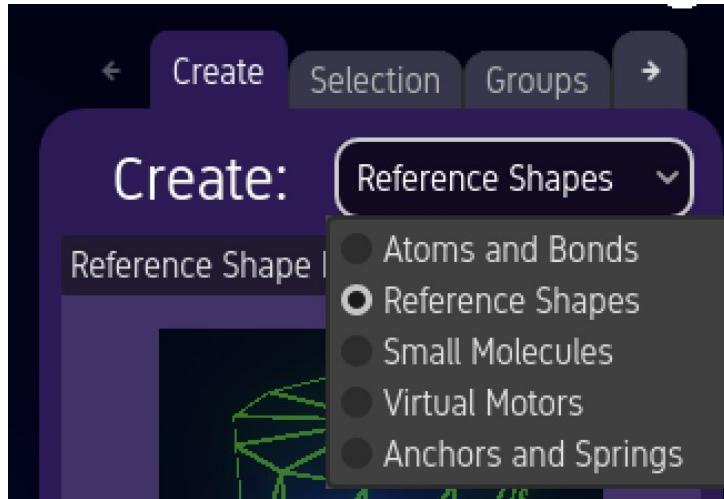
- From the Ring Menu, go to the Reference Shapes submenu...



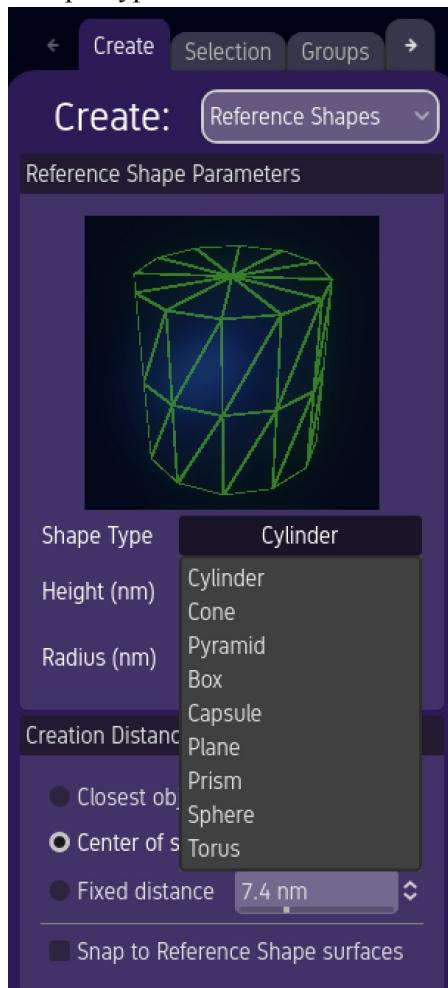
- ...then, from the Ring Menu, choose the type of Shape you'd like to create.



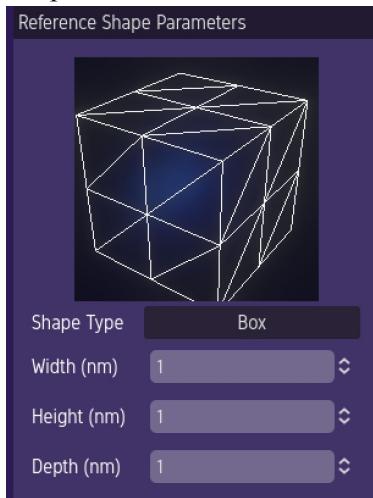
- c. You can also choose Reference Shapes from the Feature Window by going to the Create panel and selecting “Reference Shapes” from the pull-down menu.



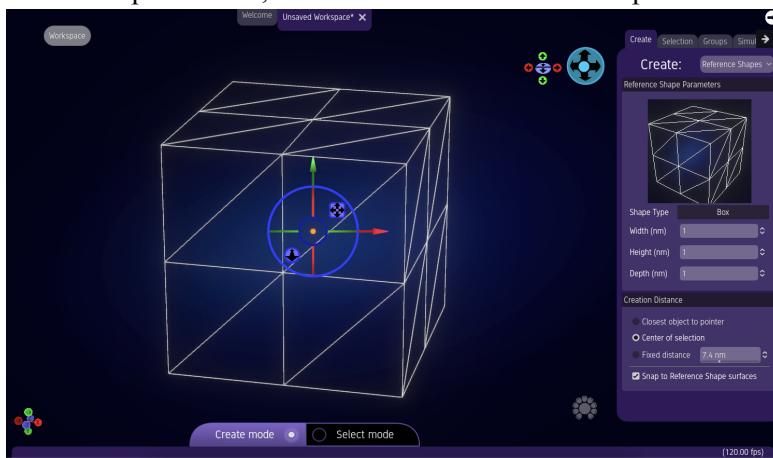
- d. In the Feature Window, choose the desired reference shape from the pull-down Type “Shape Type” menu.



- e. Shape attributes can be edited in the “Create” Feature Window.

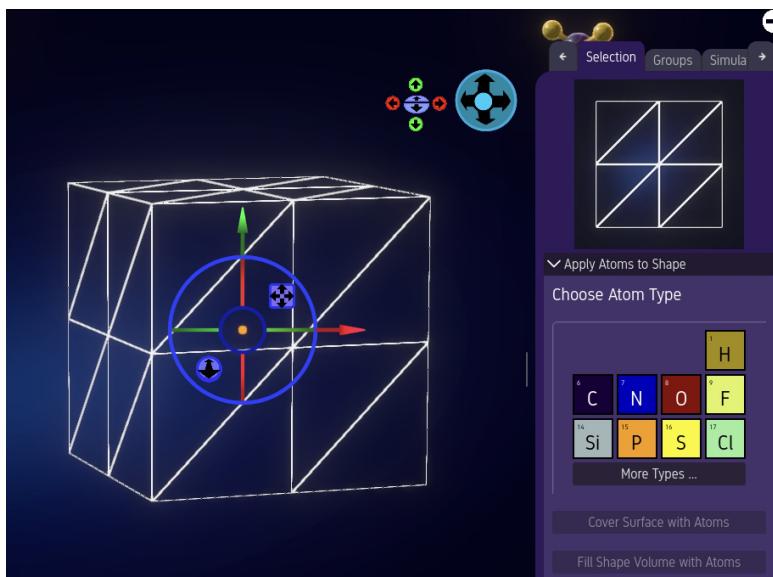


- f. With a shape selected, click in the Editor Window to place the selected Shape.



5. Applying Atoms to Shapes

- a. You can automatically place atoms around the surface of a shape, or even fill a shape with atoms.



- b. Create and Select a Shape
c. In the Selection Tab, expand the “Apply Atoms to Shape” panel.

- d. Select the Atom Type you'd like to use.

✓ Apply Atoms to Shapes

Choose Atom Type

			1 H
6 C	7 N	8 O	9 F
14 Si	15 P	16 S	17 Cl

More Types ...

Minimum Distance

Atomic Diameter

Equilibrium Distance

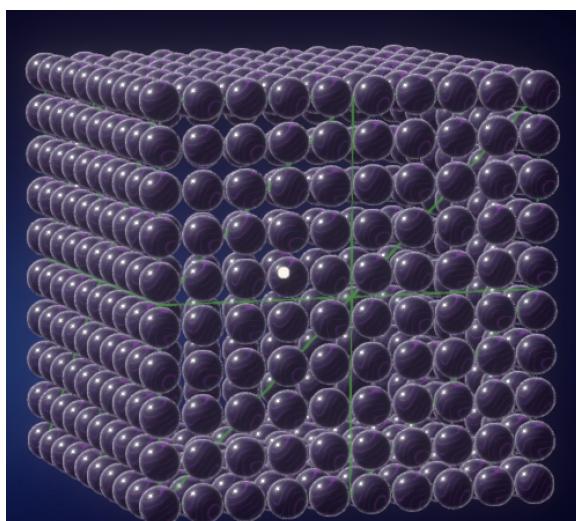
0 nm

Cover/Fill whole shape

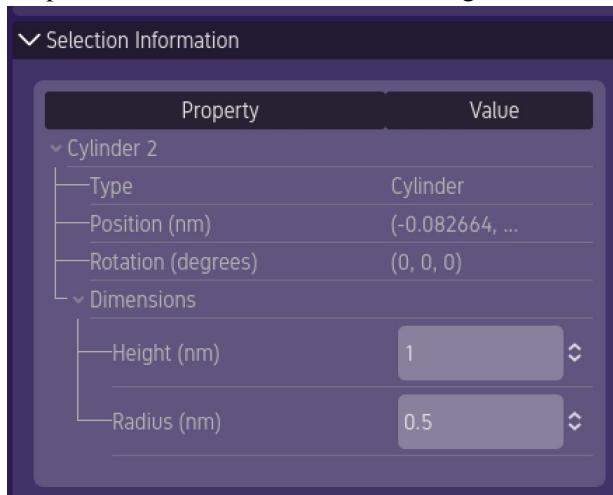
Cover Surface with Atoms

Fill Shape Volume with Atoms

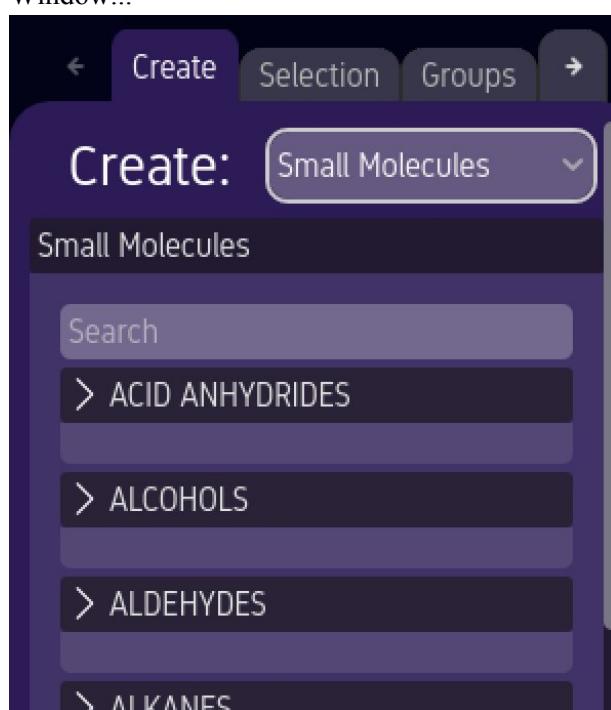
- e. To cover the surface of the shape with the selected atom type, press ‘Cover Surface with Atoms’.



- f. To fill the shape's volume with the selected atom, press 'Fill Shape Volumes with Atoms'.
6. Once a reference shape is created, its properties can be edited in the Selection tab. First, select the shape. Then in the Selection Tab, change its attributes.



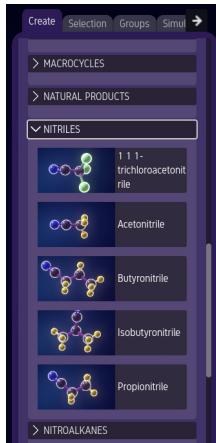
7. Creating Small Molecules
- a. Small Molecules are commonly used molecules. MSEP.one contains a library of Small Molecules. You can access this library either from the "Create" tab of the Feature Window...



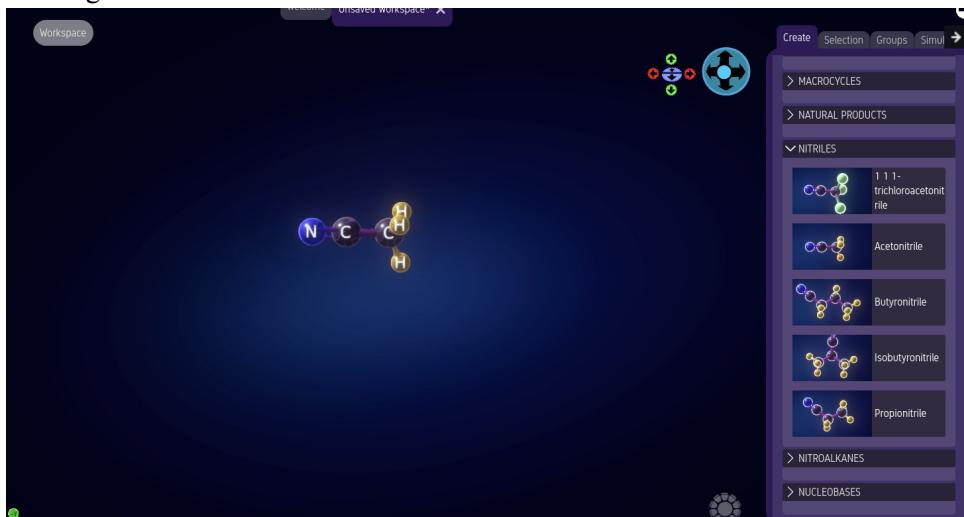
- b. ...or the File>Small Molecule Icon in the Action Ring.



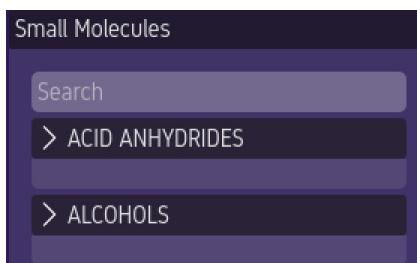
- c. In the “Create Small Molecules” Feature Window, expand a Fragment Type header by clicking.



- d. Then click on the icon representing the fragment you'd like. Next, create the fragment by clicking in the Editor Window.

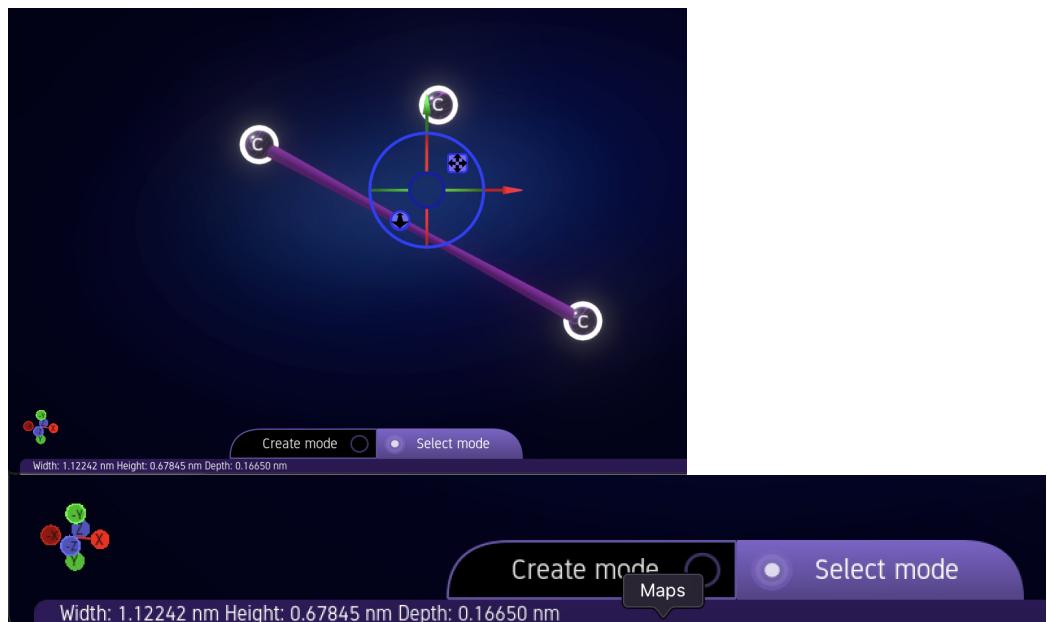


- e. To search for a specific molecule in the list of small molecules, type its name in the Small Molecule Search bar.



8. Measurement Tool

- a. You can measure objects in the Editor Window by selecting them. The dimensions of the selection will appear in the Message Bar at the bottom of the application.



9. Point-of-View Camera Movement

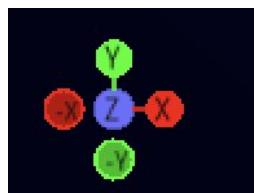
- When the Editor Window contains at least one object, you can adjust its Point-of-View (POV) Camera.
- To translate the POV Camera use the buttons in the “Camera Translation Gizmo.” The red arrows will move the camera in the X-Axis (side to side). The green arrows move the camera in the Y-Axis (up and down). The blue buttons move the camera in the Z-Axis (forward-and-back).



- Press and hold one of these buttons for continuous motion.
- To move the camera more rapidly, press and hold the <SHIFT> key while using the “Camera Translation Gizmo.”
- To rotate the camera around a fixed object, select the object, then use the “Camera Rotation Gizmo.” Press and hold the gizmo, then pull the mouse in the direction you’d like the POV camera to rotate.



- When creating a new Workspace, MSEP.one assigns an initial orientation for the project’s X, Y, and Z-Axis. You can reset the camera’s POV to one of these axis with the “Snap-to-Axis” gizmo in the lower-left-hand corner of the Editor Window. Click on one of the gizmo’s colored circles and the camera POV will move until it is parallel with the desired axis.



- You can drive the POV camera with keyboard controls.

- i. 'w' is Forward
 - ii. 's' is Backward
 - iii. 'a' is Translate Left
 - iv. 'd' is Translate Right
 - v. 'q' is Translate Up
 - vi. 'e' is Translate Down
 - vii. Hold the <SHIFT> key while using the keyboard controls to increase camera speed.
10. Selecting and Deselecting Objects in the Editor Window

- a. Click on the object you would like to select.

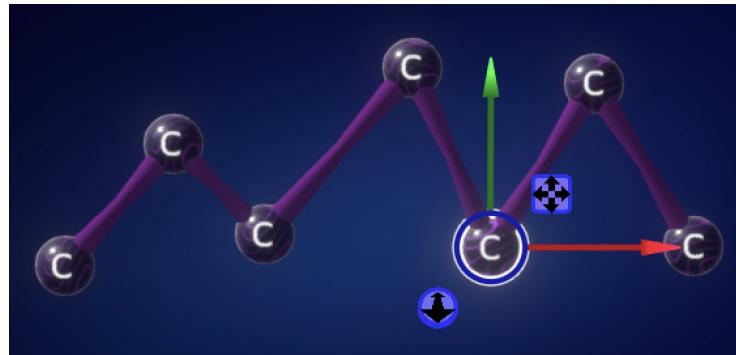


- b. To select multiple objects simultaneously, press and hold the <SHIFT> key while clicking on **unselected** objects.

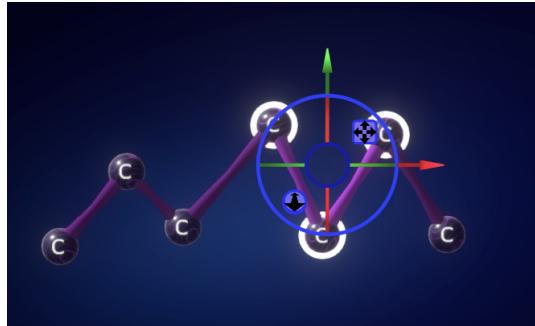


- c. To toggle the selection state of an object from a Selection Set, hold the <SHIFT> key while clicking on already **selected** objects.
- d. To remove a selected object from a Selection Set, press <CNTL> or <CMD> then click on the object you'd like to remove.
- e. You can also select multiple objects by drawing a box around them. Start by clicking on an empty space in the Editor Window. Hold down the mouse button and drag the cursor so it draws a box. When you release the mouse button, any object within the box will be selected.
- f. When a bonded object is selected, you can grow the selection so it includes some or all of the connected atoms.

- i. Select the first Atom.



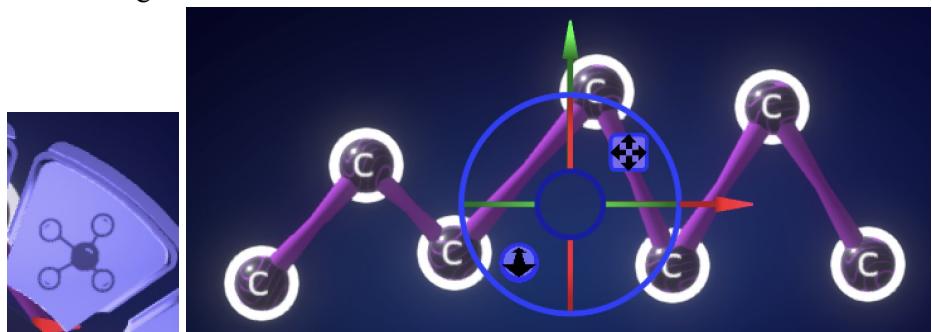
- ii. To grow the selection, press the ‘+/-’ key.



- iii. You can also grow the selection from the Selection submenu of the Action Ring.



- iv. To select all Atoms connected by Bonds, use the “Select Connected” icon in the Action Ring->Selection submenu.



- v. To shrink a Selection, press the ‘-’ key, or use the “Shrink Selection” icon in the Ring Menu’s Selection submenu.



- g. To Select All objects in the Editor Window use the “Select All” icon from the Ring Menu’s Selection submenu. On Mac, press “Command+A”



- h. To invert a Selection, use the Invert Selection icon in the Selection submenu of the Action Ring.



- i. To deselect all, either click in an empty area of the Editor window, or use the Deselect All icon in the Action Ring’s Selection submenu.



11. Selected Object Transform Gizmo



- a. When you select objects in the Editor Window, the Object Transform Gizmo appears. This control allows you to move the Selected Objects.

- i. Horizontal/Vertical Translation Control



- 1. To move the selected objects Left/Right or Up/Down in the Editor Window, click and hold on the Translation Control button, then drag the selected objects to the desired screen location. Then release the mouse button to drop the selected objects at their new location.

- ii. Z-Depth Translation Control



- To move selected objects in the Z-Axis, click and hold on the Z-Depth Translation control. Move the cursor up to push the objects away from the camera. Pull the cursor downwards to pull the object toward the camera.

iii. Rotation Rings



- The Rotation Rings allow you to rotate selected objects around their central point.
 - To rotate selected objects around the X axis, click and hold the red line within the blue circle. While holding down the mouse button, move your cursor. Release to place the objects.
 - To rotate selected objects around the Y axis, click and hold the green line within the blue circle. While holding down the mouse button, move your cursor. Release to place the objects.
 - To rotate selected objects around the Z axis, click and hold the blue circle. While holding down the mouse button, move your cursor. Release to place the objects.

2. 15 Degree Increments

- You can rotate selected objects in 15 degree increments by holding down the SHIFT button while you click and drag on one of the Rotation Rings.

iv. Horizontal Movement Arrows



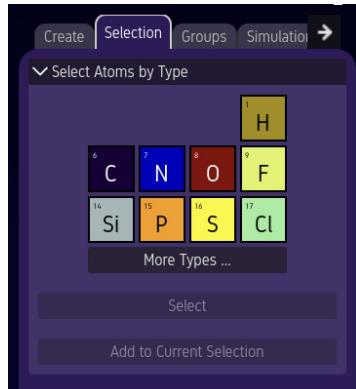
- To move selected objects only in one direction, click on one of the Horizontal Movement Arrows and drag.
 - Click and drag on the green arrow to move selected objects in the screen's Y axis.
 - Click and drag on the red arrow to move selected objects in the screen's X axis.
- By holding down the Shift Key and clicking and dragging on the Horizontal Movement Arrows, you will constrain the the objects you have selected so that they move only in the axis of those arrows.

12. Deleting Objects from the Editor Window

- Select the desired object or objects
- Press the <DELETE> key or...
- From the Action Ring's Edit Menu, select the Delete icon.



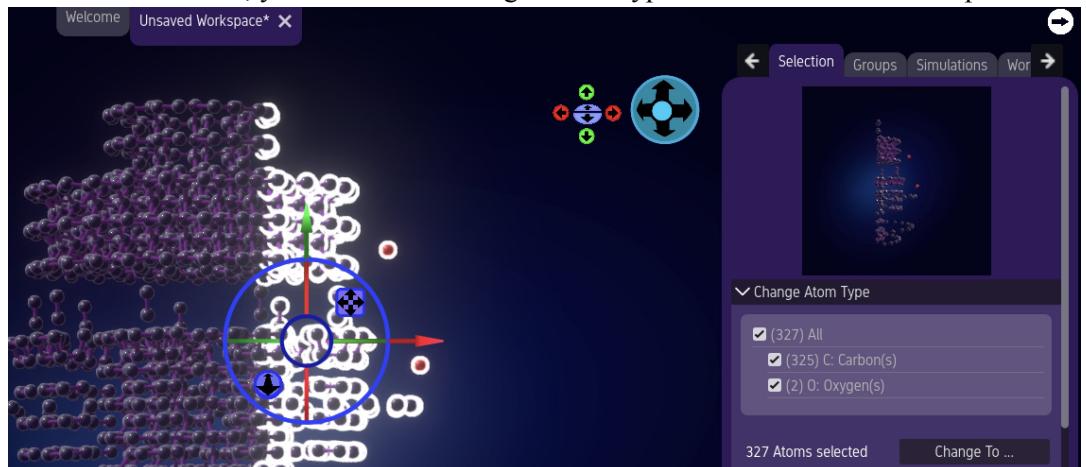
- d. To select Atoms by their specific types, use the “Select Atoms By Type” panel in the Feature Window’s Selection tab.



- From this panel, click on the Atom Types you’d like to select. Or you may click on the “More Types...” button to access the “Interactive Periodic Table” and select Atom Types there.
- Once you have selected the desired Atom Types, you can click the “Select” button to select only those Atom Types, or click “Add to Current Selection.”
- To clear your chosen Atom Types, press the “Remove Selection Filters” button.

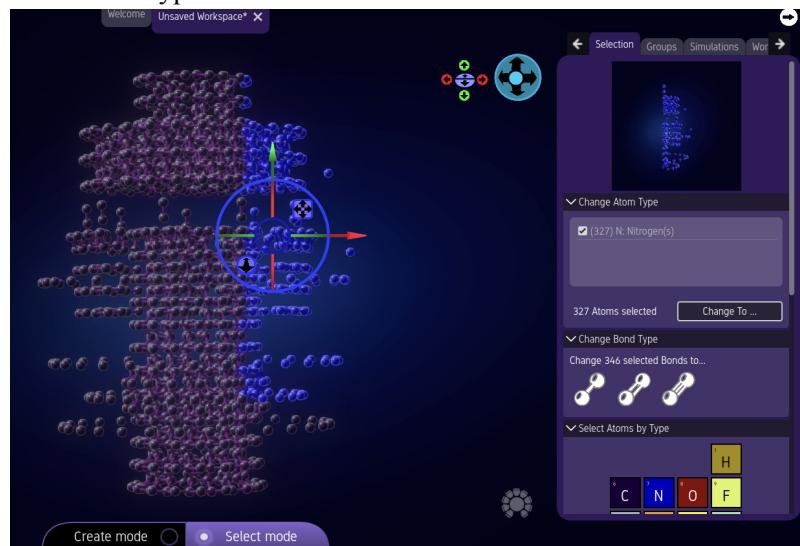
13. Swapping Atom Types

- MSEP.one allows you to swap the Atom Types of existing atoms with new Atom Types.
- First, select the group of atoms you’d like to modify.
- In the Selection Tab, you will see a “Change Atom Type” header. Click this to expand it.



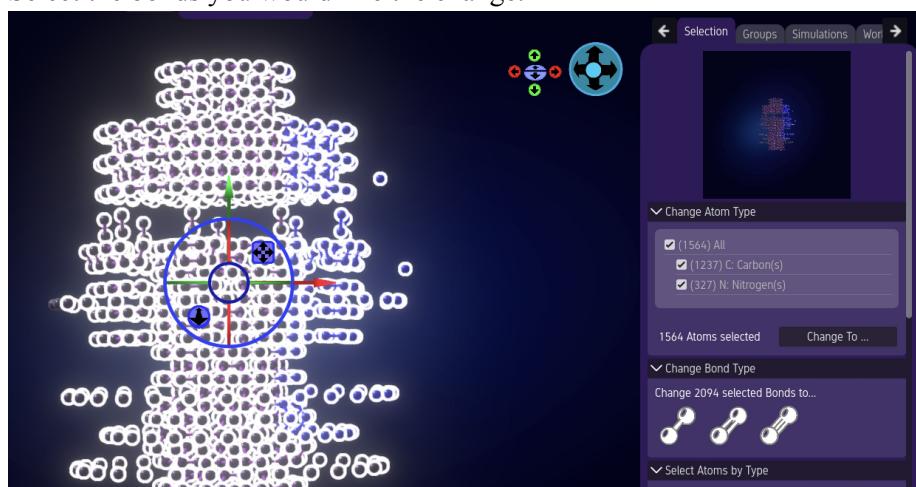
- In the Change Atom Type panel is a list of all the Atom Types in the selection. Check or un-check the items in the list, so that only Atom Types you’d like to modify are checked.
- Click the “Change To...” button.
- An Atom Picker will pop up. From it (or the associated “Interactive Periodic Table”) choose the Atom Type you would like to replace the selected list items. This will switch the selected atoms of the desired types to be replaced with the

new Atom Type.

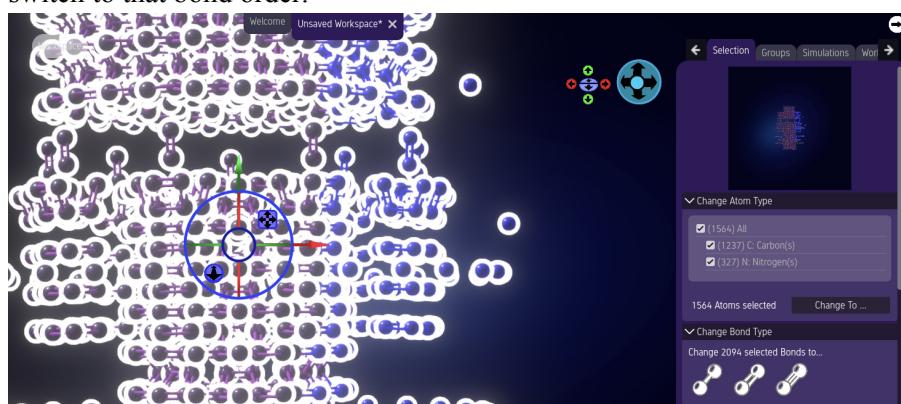


14. To change the Bond Orders of multiple, selected bonds:

- Select the bonds you would like the change.



- In the Selection Tab, expand the “Change Bond Type” header.
- When you click on the single, double, or triple bond type icons, every selected bond will switch to that bond order.



15. View Menu

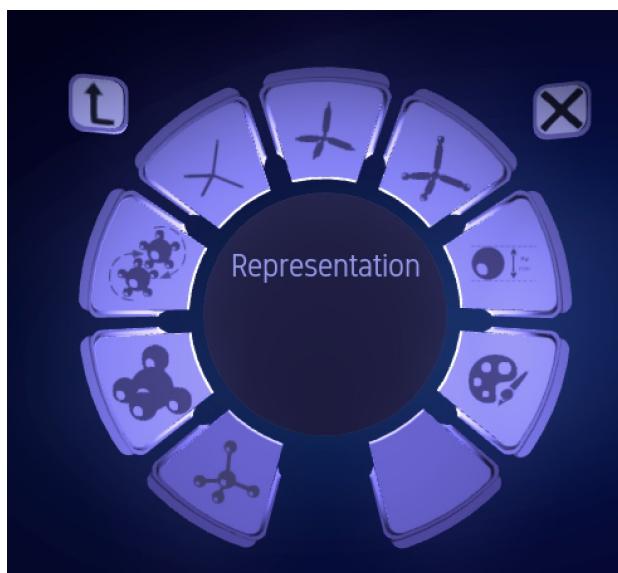
- Features in the View Menu control how the program displays objects in the Editor Window.
- Focus on Visible Objects



- i. Choosing this Icon centers all objects in the Editor Window and zooms the camera so that they are all accessible.
- c. Focus on Selected Objects



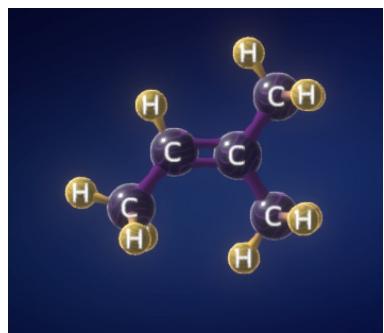
- i. This feature centers and zooms the Editor Window camera on objects that are selected.
- d. Representation Menu
 - i. Within the View menu is the Representation Icon. Clicking this icon takes the Action Ring to the Representation Menu. From this menu, users can select how atoms are rendered in the Editor Window.



- ii. Ball-and-Stick Icon



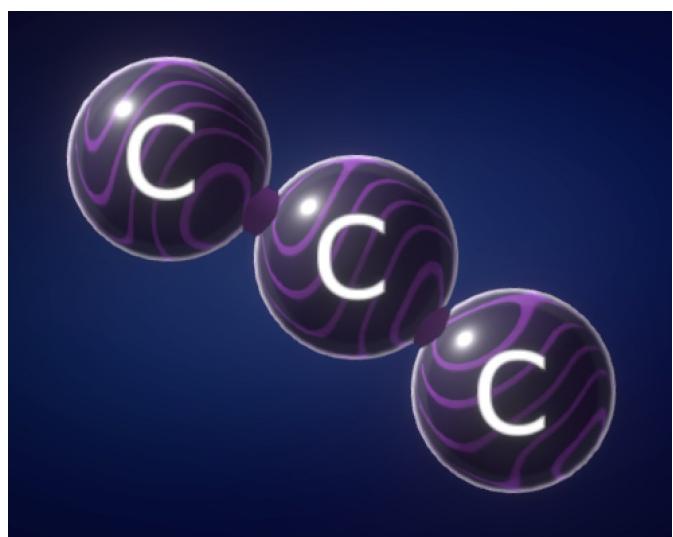
- 1. Click this to show structures in the Editor Window as Atoms and Bonds. This is the default view.



iii. Van der Waals



1. Click this icon to view atoms in their Van der Waals diameters.



iv. Mechanical Simulation Representation

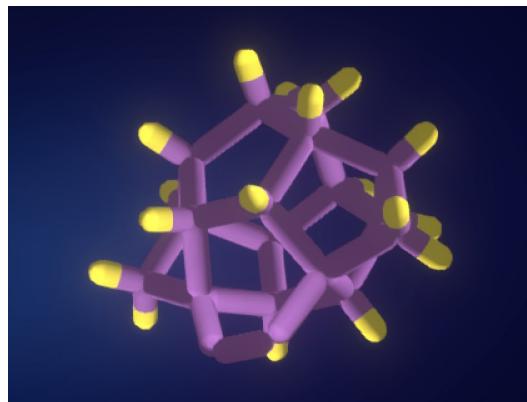


1. This representation approximates the atomic diameter at which the atoms will mechanically push each other.

v. Sticks



1. Pressing this icons renders atoms and bonds as “Sticks.”



vi. Enhanced Sticks



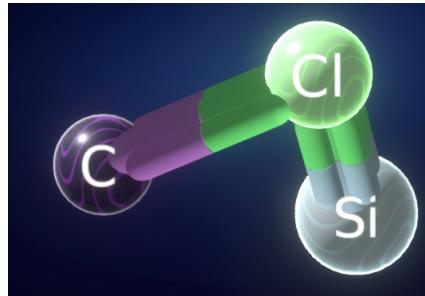
1. The Enhanced Sticks view is similar to the Sticks View, except that it additionally represents bond orders. When fully implemented, this view will be able to represent partial bond orders.



vii. Enhanced Balls-and-Sticks



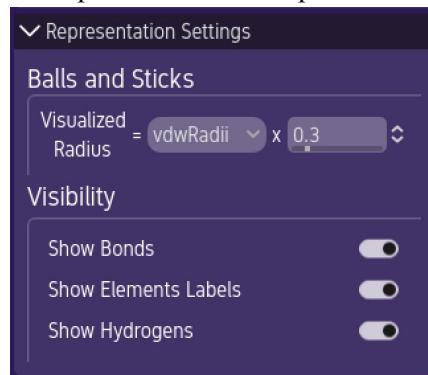
- The Enhanced Balls-and-Sticks view is similar to the Balls-and-Sticks representation, except that it additionally represents bond orders in a different fashion. When fully implemented, this view will be able to represent partial bond orders.



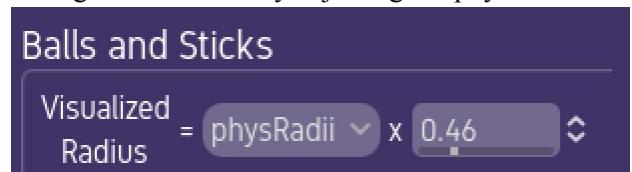
viii. Balls-and-Sticks Size Settings



- By choosing this icon, the user can manually set the size of atoms and bonds in the Balls-and-Sticks visualization. Editing the value takes place in the Workspace Settings panel.



- Change the Atom diameter by selecting and changing the vdwRadii.
- Change bond widths by adjusting the physRadii value

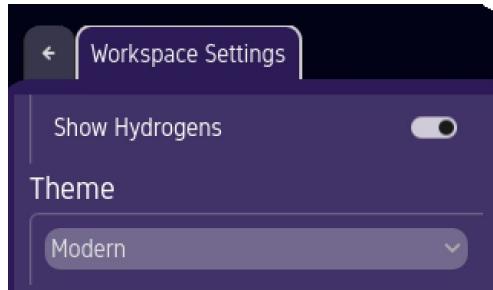


ix. Theme

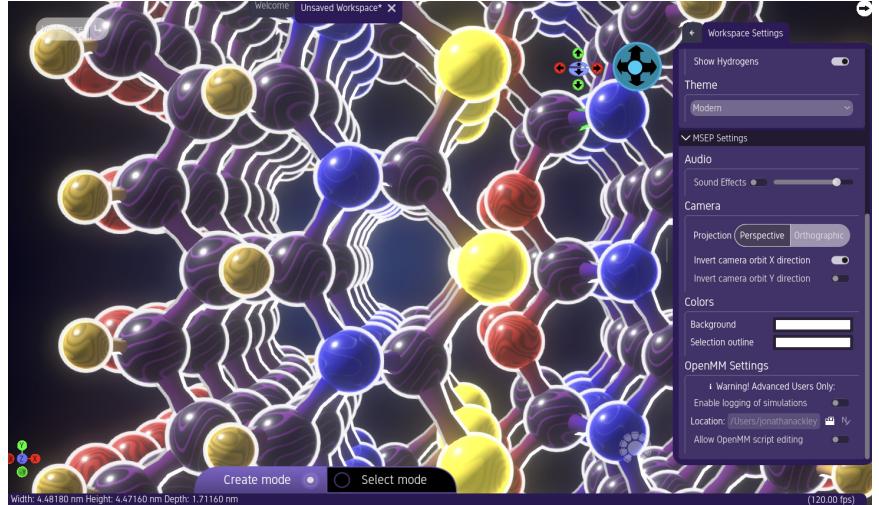


- It is simple to change the entire look and feel of the application by changing the Theme setting. It can be set in the Workspace tab of the

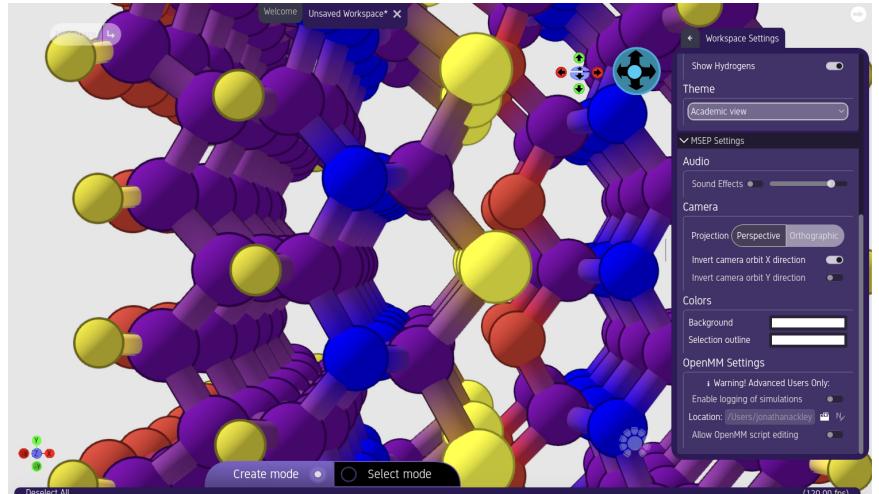
Features Window, and is also accessible from the Action Ring:
View->Representation->Theme



2. MODERN is the default setting. It is animated and color-coordinated.

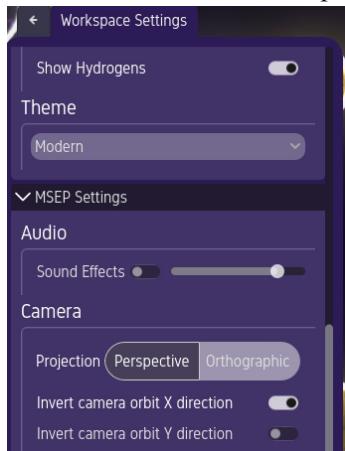


3. ACADEMIC VIEW renders projects in the fashion traditionally used in scientific, or academic papers.



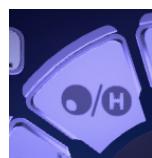
- e. Virtual Camera Settings - Perspective and Orthographic Camera Settings
 - i. You can change the editor so it displays projects in Perspective or Orthographic Projection views. These controls are found in the Workspace tab of the Features

Window, in the “Camera” panel.

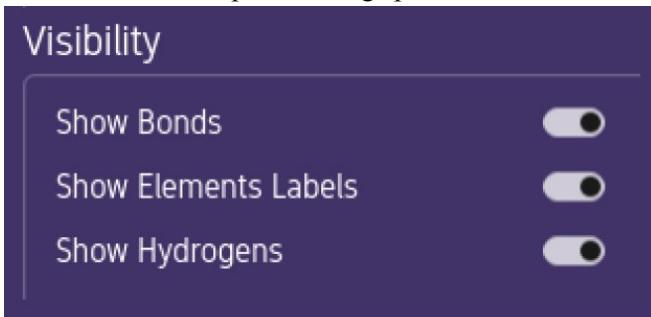


1. The default Projection setting is “Perspective.” In the Perspective setting, MSEP.one renders the project as though it had depth. Objects further from the camera converge toward a Vanishing Point.
2. The Orthographic Projection does not attempt to illustrate object depth. All objects are rendered as if they are the same distance from the camera.

f. Show / Hide Element Labels Toggle



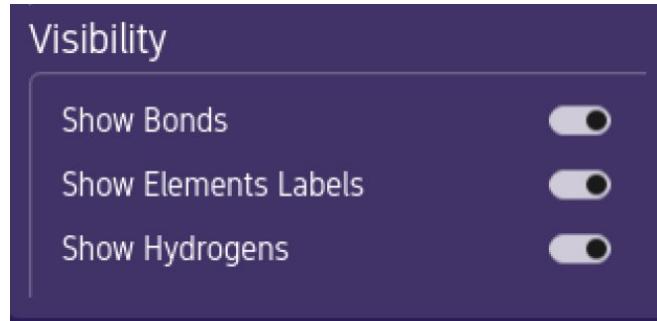
1. Click this to toggle the visibility of the Element Labels on atoms. The toggle is found in the Workspace Settings panel.



g. Show / Hide Bonds Toggle



1. Allows users to hide bonds in the Editor Window.



- a. Show / Hide Hydrogens Toggle



1. Allows users to hide hydrogen atoms in the Editor Window.

- a. Hide Selected Objects



1. Click this icon to make all selected objects invisible in the Editor Window. These hidden objects will remain in the project and will interact with other objects during simulations, but the will not be seen.

- b. Show Hidden Objects



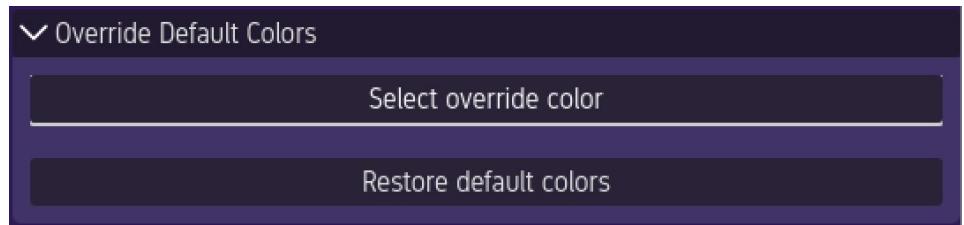
1. Selecting this icon makes all hidden objects visible again.

- c. Override Default Colors

2. The user can arbitrarily change the colors of atoms.
3. From the "View" menu of the "Action Ring" select "Override Default Colors."



4. Select the atoms whose colors you would like to change.
5. From the "Override Default Colors" Panel in the "Selection Tab" choose "Select Override Color".



6. A “Color Picker” interface will pop up. Use this tool to select the desired color.



7. When you have chosen a color, hit the ‘Apply’ button. All selected atoms will change to this color.
8. To restore overridden atoms to their original colors, select them and press: “Restore default colors” in the “Override Default Colors” Panel in the “Selection Tab.”

- a. Image Capture and Export

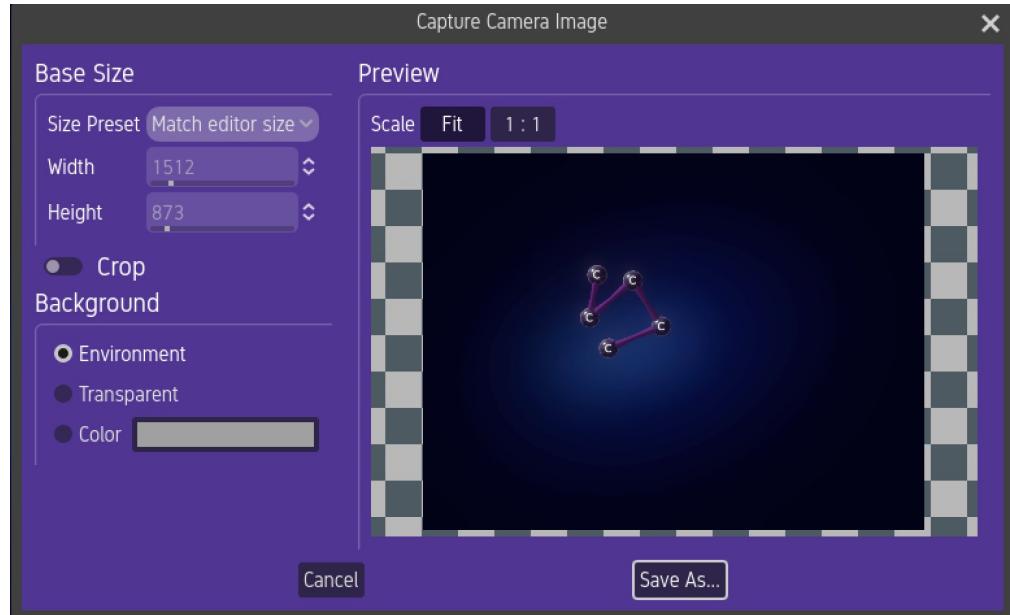
1. MSEP.one allows you to save images of your project.
2. First, frame your project using the POV Camera.
3. Next, from the View Menu of the Action Ring, select the Camera Icon to move into the Camera Menu.



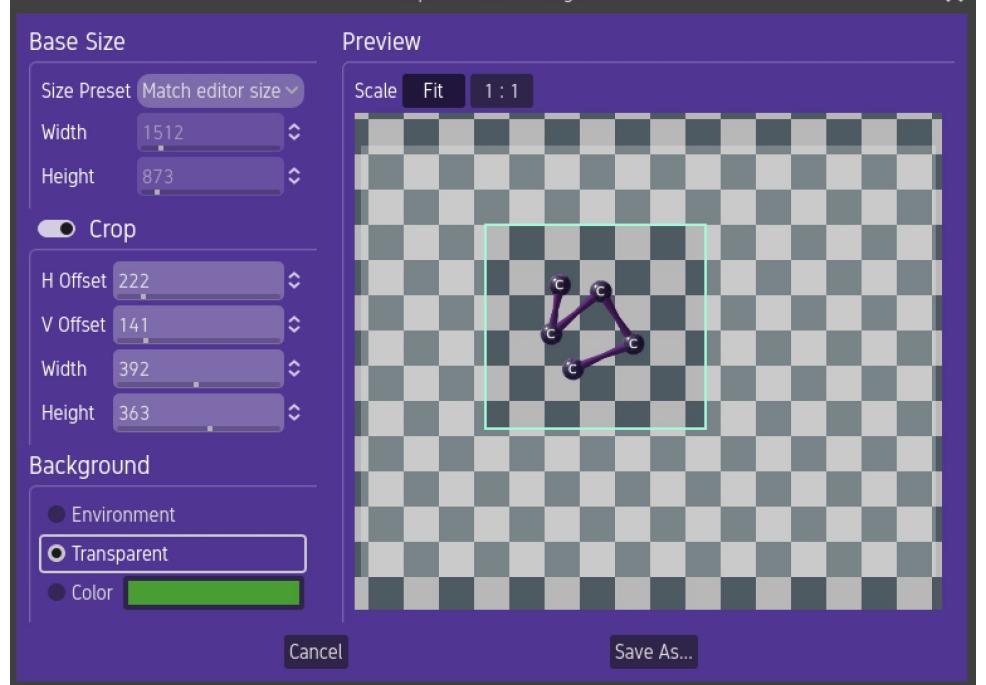
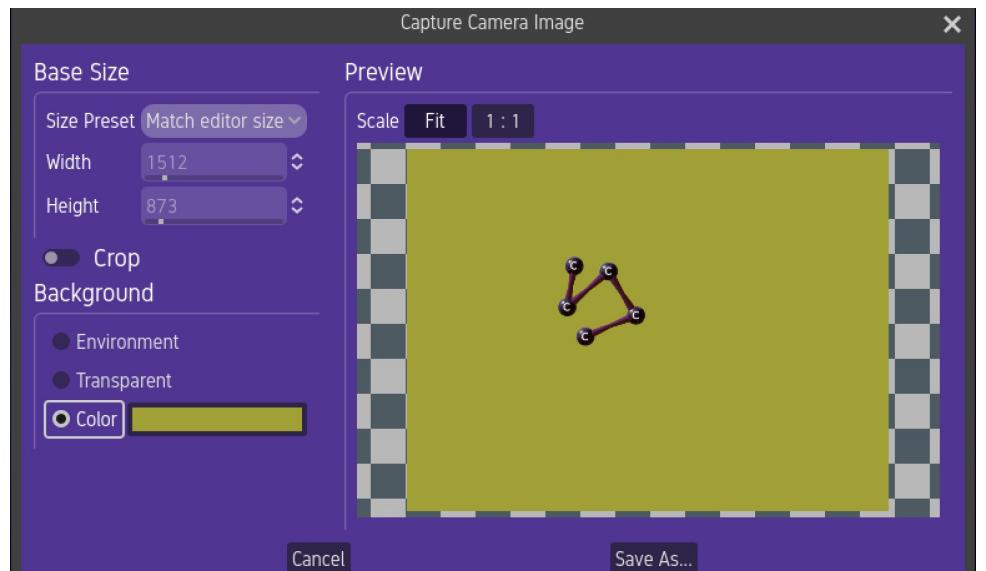
4. Capture Camera Image icon in the Camera submenu.



5. This brings up the Camera Capture Image dialog.



6. Here, you can change the color of the image background. Background color can also be made transparent.



7. You can crop, scale, or change the output resolution of your image.



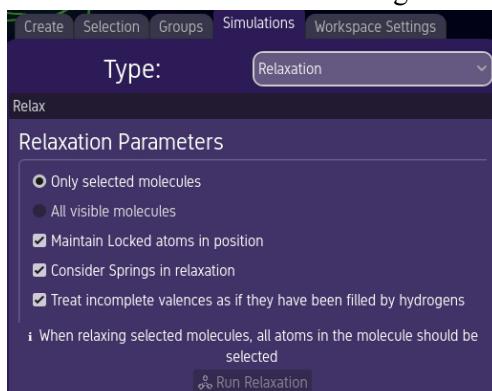
16. Running Simulations

a. Relaxation

- To access Relaxation, raise the Action Ring and select the Relaxation Icon in the Simulations submenu.

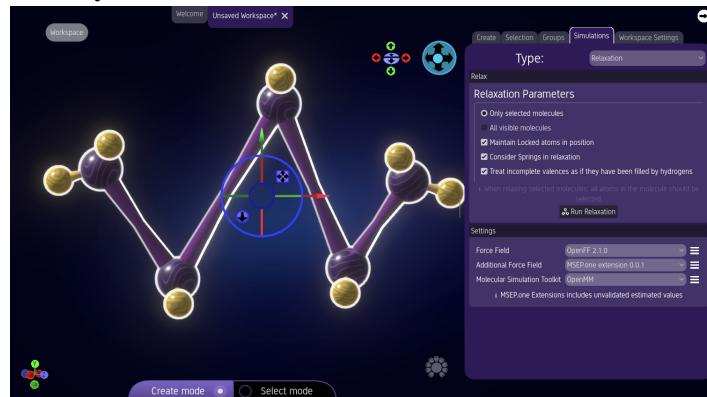


- You can also find the Relaxation simulation by going to the Simulations tab in the Feature Window and selecting “Relaxation” from the Type pull-down menu.

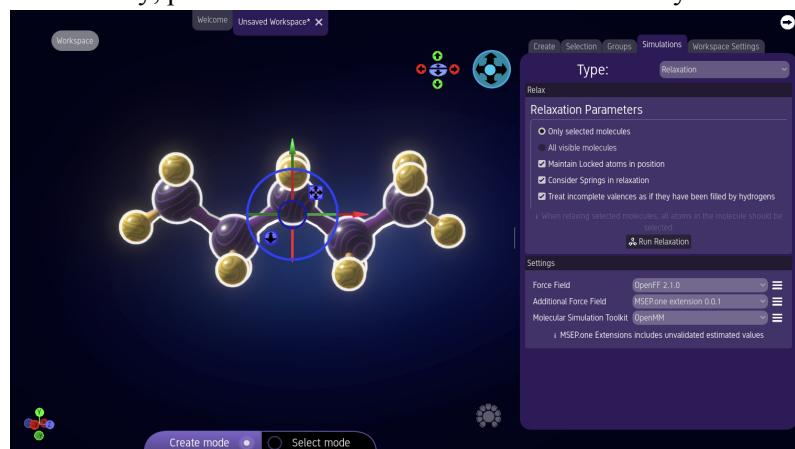


- From the “Relaxation Parameters” panel, choose whether you want to relax All Molecules or only Molecules that are selected.
- The Relaxation simulation cannot relax partial molecules. If relaxing “Only Selected Molecules”, the Relaxation will only succeed if the desired molecules

are fully selected.



- v. When ready, press the “Run Relaxation” button to relax your model.

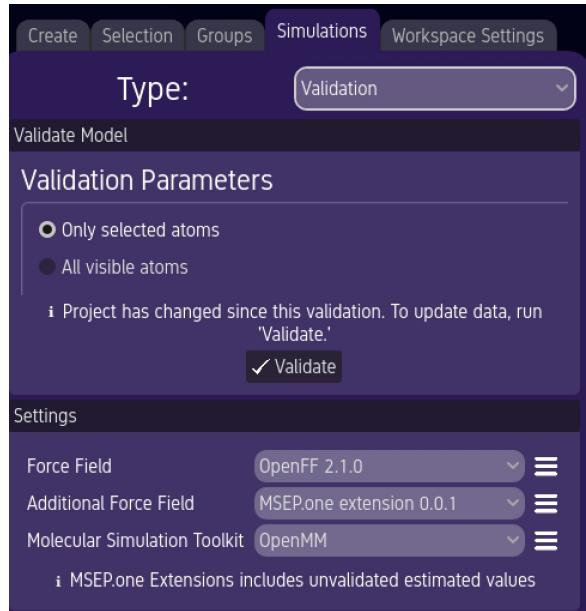


b. Validation

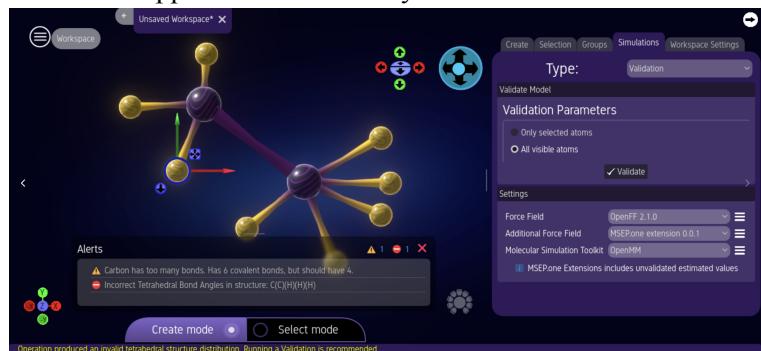
- i. This feature allows you to check your model for correctness. For example:
 1. Are there overlapping/conflicting atoms?
 2. Are the number of bonds correct?
 3. Are any springs ignored?
 4. Are there invalid tetrahedral structures?
 5. Are there bond angles outside the expected range?
- ii. Navigate to the Validate Model feature by pressing the Validate Model Icon in the Simulations submenu of the Ring Menu...



- iii. Or you can choose Validation from the Type pull-down menu in the Simulations Tab of the Feature Window.

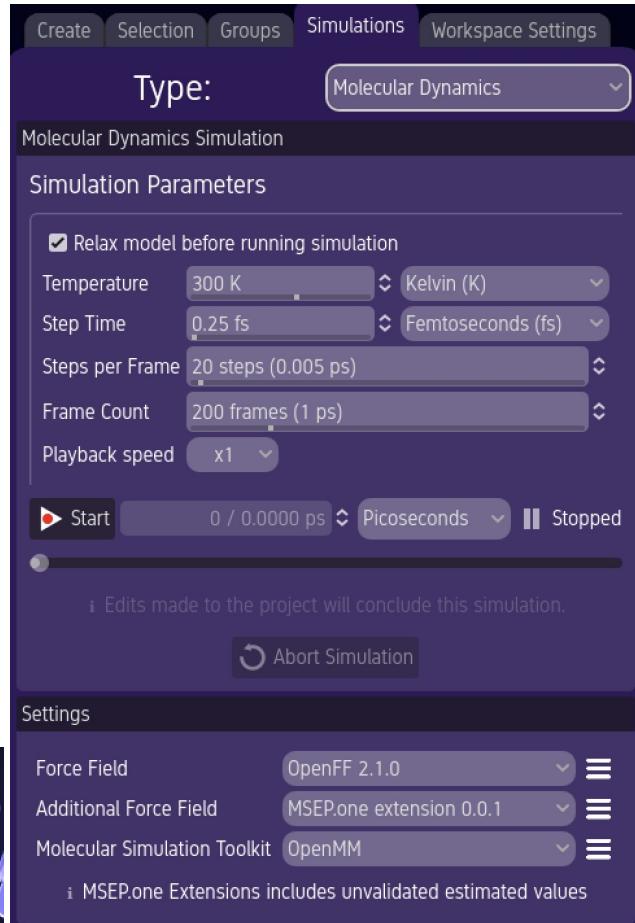


- iv. In the Validation Parameters panel, choose to validate selected atoms or all atoms.
- v. Press the “Validate” button.
- vi. Errors will appear in the Summary Panel.

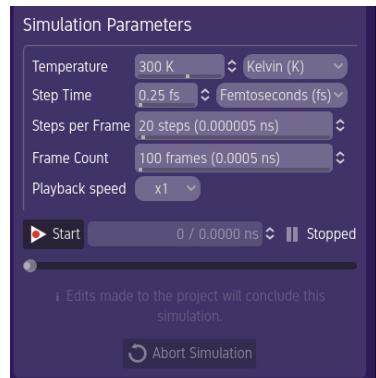


- vii. When you click on an Error in the Summary Panel, the program will automatically select the object at issue.
- c. Molecular Dynamics
 - i. Access the Molecular Dynamics Simulation feature by either using the “Molecular Dynamics” Icon in the Action Ring’s Simulation sub-menu, or the

Type pull-down menu in the Simulations tab of the Feature Window.



- ii. Customize the values in the Simulation Parameters panel.



- iii. When ready, press the “Start” button.



- iv. Depending on the size of the model, there may be a delay before the simulation begins playback.
- v. After completing initial calculations, the simulation will begin to play. As it plays, you may use the Camera POV controls to view the simulation from different views.
- vi. You can control Simulation Playback with the Playback Controller.

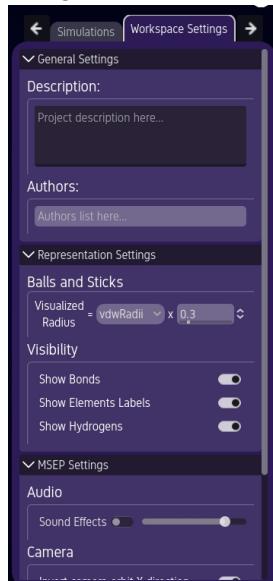


- vii. To save changes made by the Molecular Dynamics Simulation, move the Playback Controller's thumb to the desired position, then begin editing the model.
- viii. If you wish to abandon changes made by the Molecular Dynamics Simulation, press the “Abort Simulation” button.

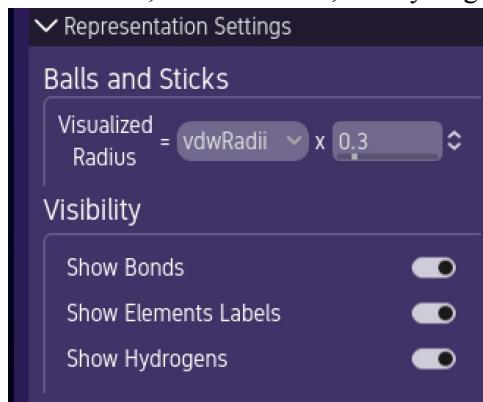


17. Customizing a Project’s Workspace

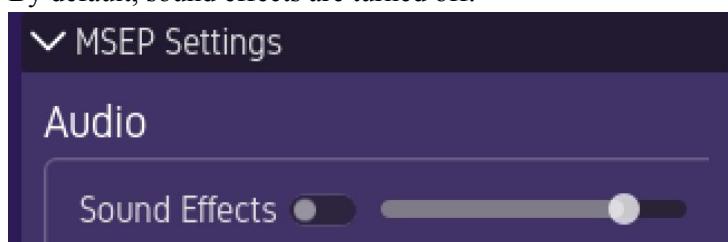
- a. You can customize your selected Workspace through the “Workspace” tab in the Features Window. Under general settings, you can enter a description of your project, along with the names of the project’s authors.



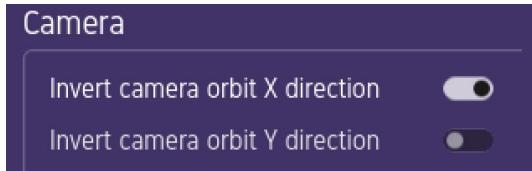
- b. Under “Representation Settings” you can change the size at which atoms are rendered in the Ball-and-Stick visualization. With the Visibility settings, you can choose whether to show bonds, element labels, and hydrogens.



- c. Under MSEP settings, you can control sound volume and turn sound effects on and off. By default, sound effects are turned off.

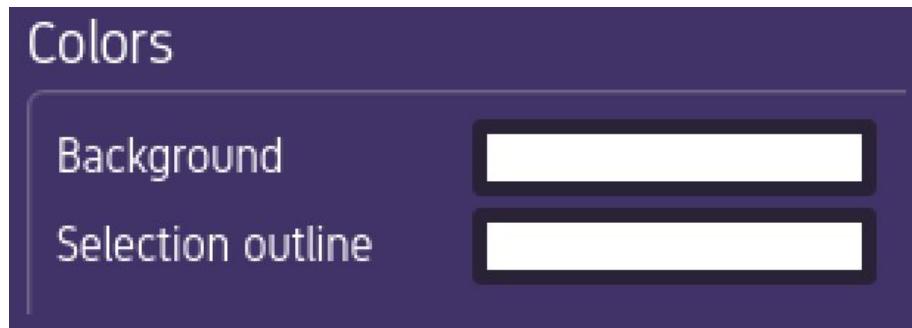


- d. If you choose, you can invert the rotational control scheme for the POV Camera.



- e. Background Colors

- i. You can customize the Background Color of your workspace with the Colors Panel.



- ii. Click on "Background" to bring up a color picker. When you have chosen a color, press "Apply." If you decide you don't want to change the background, click away to dismiss the color picker. To restore the Workspace to its default background, press "Reset."



18. File Options

- a. These File Options are found in the Action Ring under the File Icon.



- b. Create New Workspace

- i. To create a new Workspace, press the New Workspace Icon.



- ii. To open a previously saved MSEP.one workspace, press the “Open Workspace” icon. Then locate the desired file in the application’s file browser.



- iii. To save your current Workspace, select the Save Workspace Icon.



- iv. If you have saved your current Workspace, you can create a named copy using the “Save Workspace As...” feature.



- v. MSEP.one can import several different atom-related files using the Import File feature.



Supported formats are:

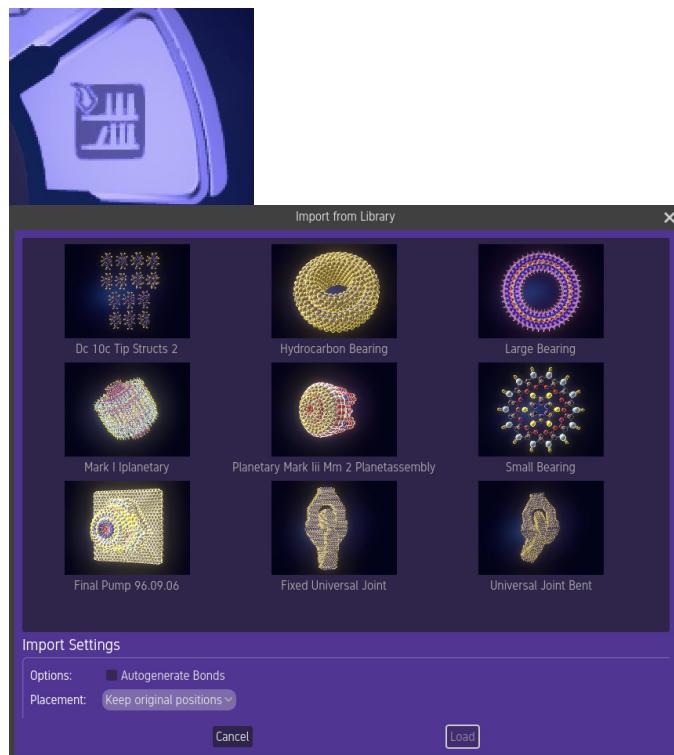
1. PDB (Protein Data Bank)
2. SDF (Structure Data File)
3. MOL (Molfile)

- vi. To export your project to a format that is not the native “.MSEP” format, click on the “Export File” icon in the “File” menu of the “Action Ring.”



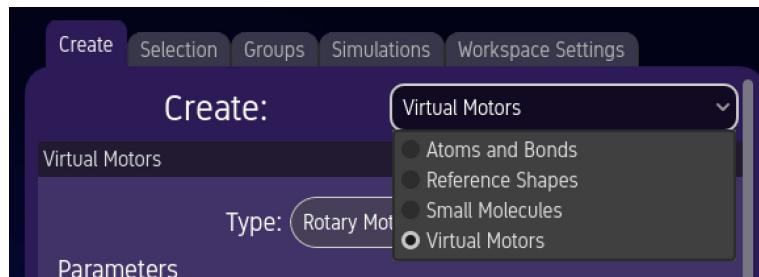
1. MSEP.one can export your project as the following file types:
 - a. PDB
 - b. XYZ

- vii. MSEP.one contains a library of prebuilt projects. These can be found by clicking the “Import From Library” icon.

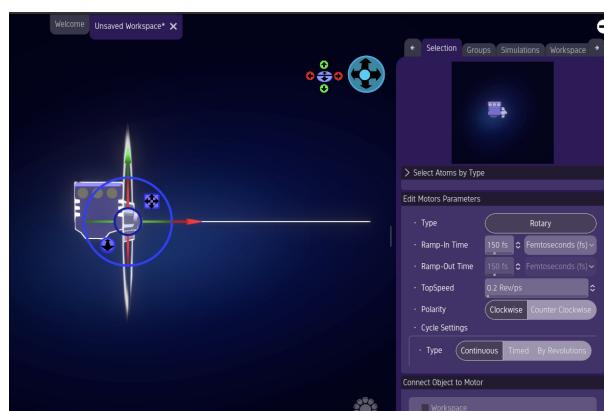


19. Virtual Motors

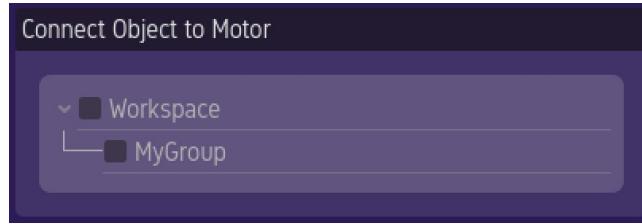
- Virtual Motors can be used to power your molecular machines.
- Please note that the Motor values have been set to extreme speeds in order to reduce simulation time. When creating your own machines, be sure to validate your motor's speed values.
- Access Virtual Motors through the pull-down menu in the Create panel.



- Virtual Motors can be attached to Groups in order to move the objects contained by those Groups. There are 2 kinds of Virtual Motors: Rotary and Linear.
- To attach a Virtual Motor to a Group:
 - Select the Virtual Motor

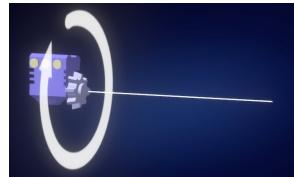


- ii. In the “Connect Object to Motor” panel, select the desired objects.

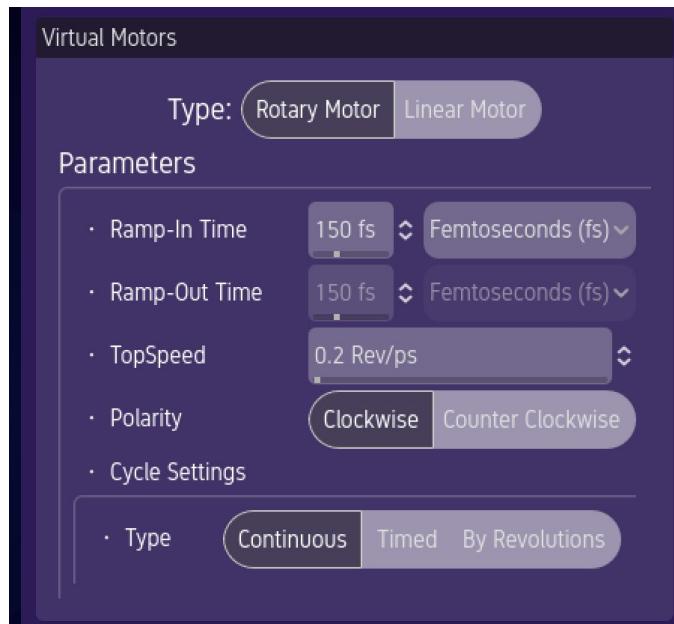


- iii. Multiple motors can be connected to the same Group.

d. Rotary Motors



- i. These motors spin objects in relation to their axis of orientation. The axis runs through the motor, exiting perpendicular to and through the center of the motor's 'spinning gear.'
- ii. An animating arrow shows the direction of the Rotary Motor's spin.
- iii. Currently, Rotary Motors support the following parameters:



- iv. Currently, Virtual Rotary Motors support the following parameters:

1. Ramp-In Time
 - a. This value defines the time it takes for the motor to go from 0 rotations-per-time-period to its maximum speed.
2. Ramp-Out Time
 - a. The time it takes the motor to go from maximum speed to 0 rotations-per-time-period.
3. Top Speed
 - a. The maximum rotations-per-time-period the motor will achieve.
4. Polarity
 - a. The direction of spin

5. Cycle Settings

Type	Continuous	Timed	By Revolutions
Move for	500 fs	Femtoseconds (fs)	
Pause for	500 fs	Femtoseconds (fs)	
Stop after	1 cycle		
Swap polarity between cycles	<input checked="" type="checkbox"/>		

a. Continuous

i. Motor cycle will run until the end of a simulation

b. Timed

i. This setting causes a motor to run for a defined period of time.

1. Move for: Here the user sets a cycle's duration time
2. Pause for: Here the user can set an amount of time to pause between cycles.
3. Stop after: The user can set the number of cycles the motor will run before ceasing to cycle.
4. Swap polarity between cycles
 - a. This feature causes the motor to reverse direction after the completion of a cycle.

c. By Revolutions

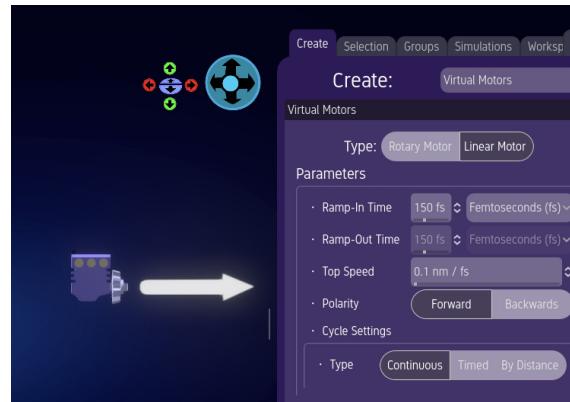
Type	Continuous	Timed	By Revolutions
Move for	1 revolutions		
Pause for	500 fs	Femtoseconds (fs)	
Stop after	1 cycle		
Swap polarity between cycles	<input checked="" type="checkbox"/>		

i. With this feature, a user can define the duration of a cycle by the number of revolutions completed by the Virtual Rotary motor.

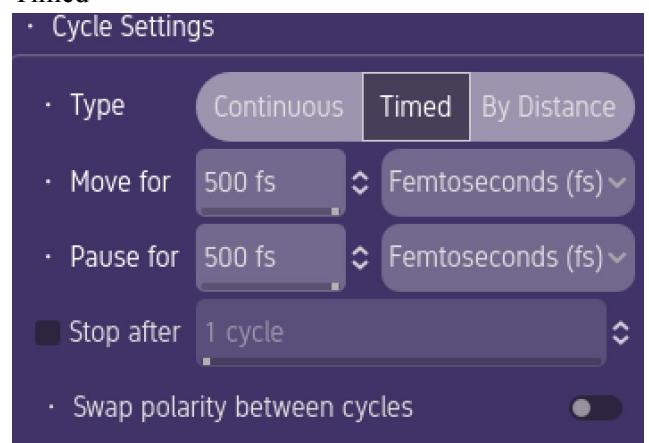
v. Linear Motors



- Virtual Linear Motors move connected objects back and forth in a straight line.
- Parameters for Virtual Linear Motors are:



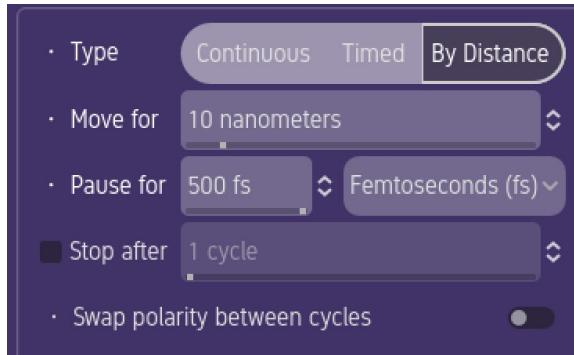
- Ramp-In Time
 - This value defines the time it takes for the motor to go from 0 to its maximum speed.
- Ramp-Out Time
 - The time it takes the motor to go from maximum speed to 0.
- Top Speed
 - The maximum speed the motor will achieve.
- Polarity
 - The direction the Virtual Linear Motor will move a connected object.
- Cycle Settings
 - Continuous
 - Motor cycle will run until the end of a simulation
 - Timed



- This setting causes a motor to run for a defined period of time.
 - Move for: Here the user sets a cycle's duration time
 - Pause for: Here the user can set an amount of time to pause between cycles.
 - Stop after: The user can set the number of cycles the motor will run before ceasing to cycle.

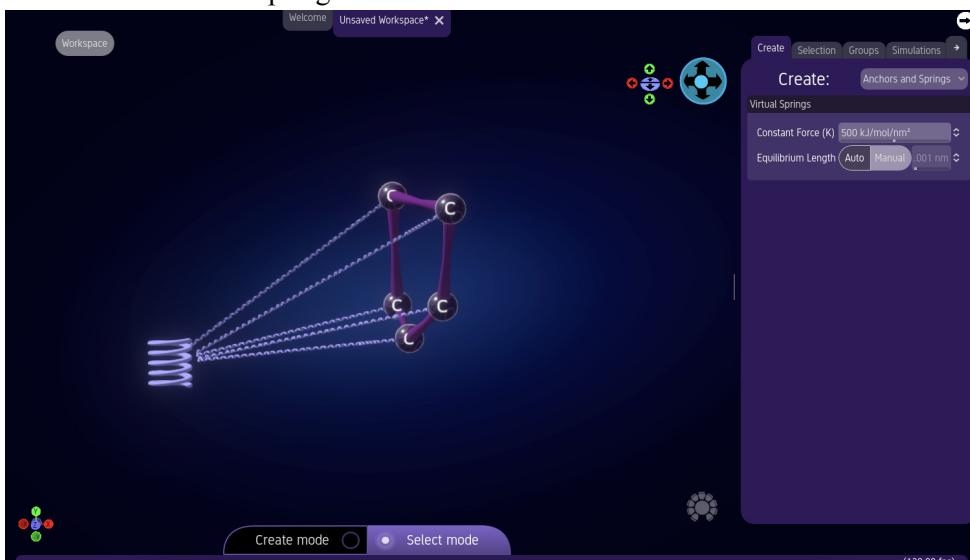
- d. Swap polarity between cycles
 - i. This feature causes the motor to reverse after the completion of a cycle.

iii. By Distance



- 1. With this feature, a user can define the duration of a cycle by the distance an object is moved by the Virtual Linear Motor.
 - a. Move for: Here the user sets the distance the Virtual Linear Motor will move an object before a cycle ends.
 - b. Pause for: Here the user can set an amount of time to pause between cycles.
 - c. Stop after: The user can set the number of cycles the motor will run before ceasing to cycle.
 - d. Swap polarity between cycles
 - i. This feature causes the motor to reverse direction after the completion of a cycle.

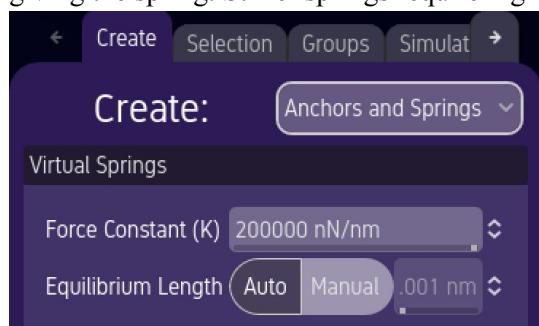
20. Virtual Anchors and Springs



- a. Anchors and bonds can constrain the motions of atoms during Molecular Dynamics simulations.
 - i. To create springs, bring up the "Anchors and Springs" option in the Create Window. You can also reach it from the Action Ring's Virtual Objects->Anchors and Springs Icon.



- ii. First set the “Constant Force” value for the spring. The smaller the force the more giving the spring. Stiffer springs require higher values. For instance: 200,000



- iii. The “Equilibrium Length” is the length of the spring when it is not under stress.
1. Use the “Auto” function to set “Equilibrium Length” to the length of the spring in the Editor Window.
 2. You can enter a custom “Equilibrium Length” value in “Manual” mode.
- iv. Select the atoms to which you would like to attach springs.
- v. To connect the selected atoms to an anchor with springs, hold down the SHIFT key and click in the Editor Window.
1. An Anchor object will appear at the point of the click. Springs will automatically connect to the selected atoms.
 2. These springs created will have the “Constant Force” and “Equilibrium Length” properties from the “Create Anchors and Springs” window.
- vi. Click and Drag
1. Can click and drag from an atom to an anchor (or vice-versa) to connect the 2 objects via a spring.

21. Groups

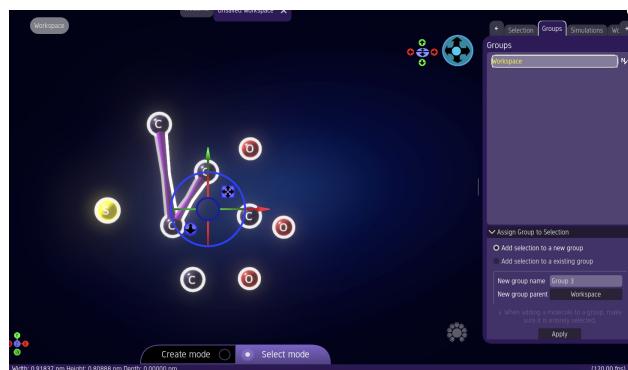
- a. Groups are collections of objects that can be treated as a single unit. For instance, a user can select a group of atoms and bonds, and then group them. By moving the group, all

objects in the group can be moved. The Groups functionality can be found in the Groups tab of the Features Window. You can easily access this tab by clicking the Virtual Objects->Groups icon in the Action Ring.

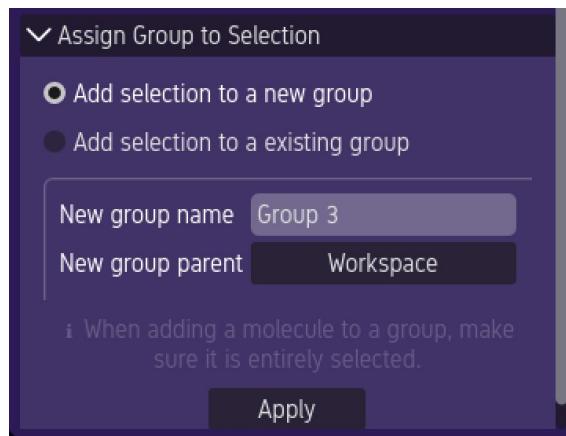


b. Creating a Group

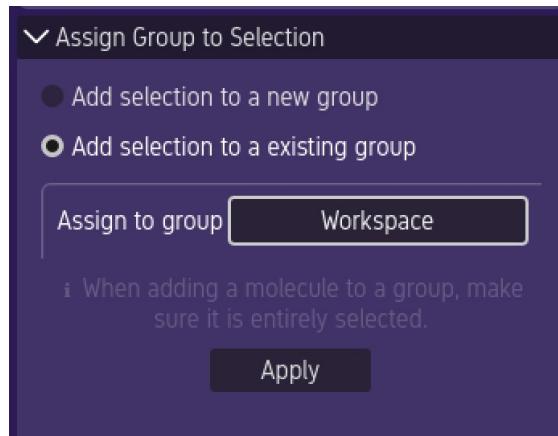
- In the Editor Window, select the objects you'd like to group.



- In the ‘Groups’ tab of the Feature Window, select the radio button, “Add selection to a new group”. You can name this group, by typing the desired name into the “New group name” field. Create the group by pressing the ‘Apply’ button.

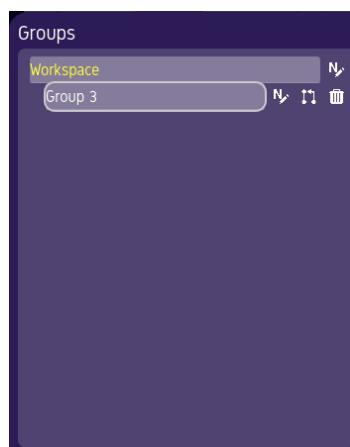


- To add a Selection to an existing group, select the objects to be combined. Next, select the “Add selection to an existing group” radio button. Choose the destination from the “Assign to group” drop-down list, then press the ‘Apply’ button.

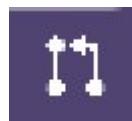


c. Dissolving a Group

- i. To dissolve a group, go to the ‘Groups’ tab of the Feature Window. At the top will be a list of available groups.

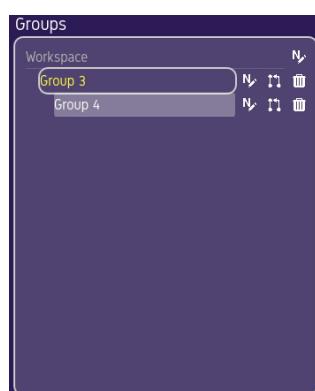


- ii. Select the group you’d like to dissolve by clicking on it. Then click on the “Merge” icon to merge the group’s objects with it’s parent.



d. Nesting Groups

- i. Groups can contain other groups. Hierarchies are represented in the Group List under the ‘Groups’ tab in the Feature Window.



- ii. Parent Groups

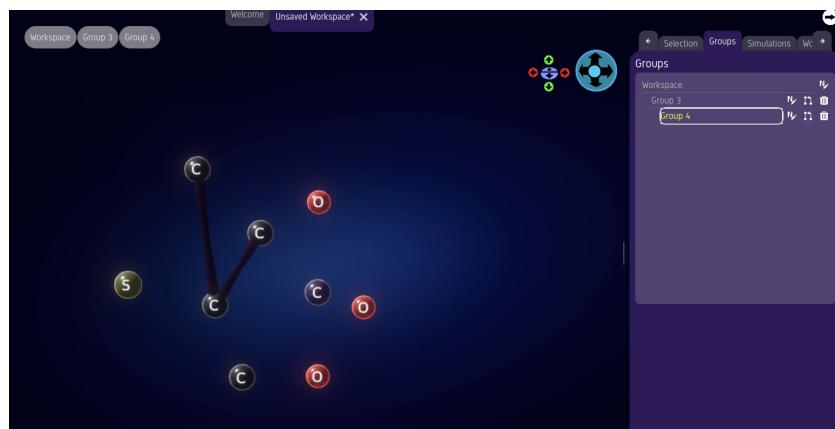
- Parent Groups appear directly above their children, which are indented to the right.

iii. Changing Group Hierarchies

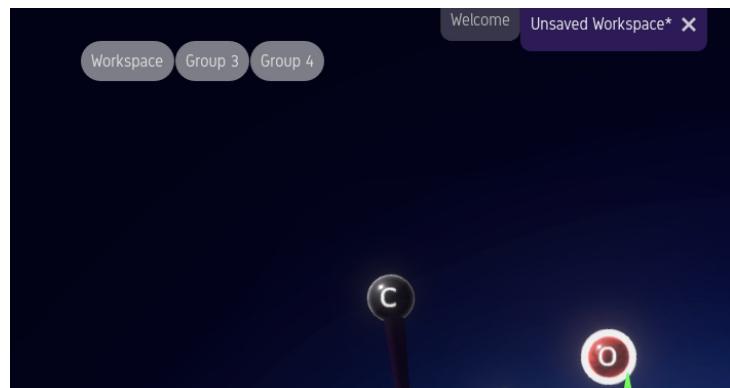
- In the Group List of the ‘Groups’ tab, the user can change group ownership. To change group ownership, click and hold on the name of the group you’re moving, then drag it to the desired position in the hierarchy. The top-level of the hierarchy is called, ‘Workspace.’

iv. Editing Groups

- To edit a group, the interface state must be ‘within’ the group you desire to edit. To enter a group, double-click on any of its member objects. You can also enter a group by double-clicking its name in the ‘Group List’ of the ‘Groups’ tab. Once ‘inside’ that group, you can edit its components.
- When a user is editing a group, only the elements of that group can be edited. Elements not contained by that group are grayed out and cannot be edited.



- The current position of the UI in the group hierarchy is displayed as a list of group names in the upper-right of the Editor Window. You can use these group name buttons for navigation. Clicking one of these buttons will move the interface state ‘within’ the selected group.



4. Deleting Groups

- To delete a group and all its contents, find its name in the ‘Group List’ on the “Groups Tab.” Then press the ‘Garbage Can’ icon next to the name.



22. Help Menu

- a. Enter the Help Menu by clicking on the Help Icon in the top-level of the Action Ring.



- b. Feature Documentation

- i. Clicking on the “Tutorials and Documentation” icon opens the latest version of MSEPt.one’s Tutorials and Documentation on your machine’s PDF viewer.



23. Keyboard Shortcuts

- a. Camera Controls

- i. Up-Arrow Key = Forward
 - ii. Back-Arrow Key = Backward
 - iii. Left-Arrow Key = Strafe Left
 - iv. Right-Arrow Key = Strafe Right
 - i. ‘w’ = Forward
 - ii. ‘s’ = Backward
 - iii. ‘a’ = Strafe Left
 - iv. ‘d’ = Strafe Right
 - v. ‘q’ = Down
 - vi. ‘e’ = Up
 - vii. To rotate the camera using the keyboard, use the above keys while holding down the OPTION key.

- b. Create Bonded Atom

- i. With atom selected, SHIFT-CLICK on an empty space in the Editor Window

- c. File Features

- i. COMMAND + ‘n’ = Create New Workspace
 - ii. COMMAND + ‘o’ = Open New Workspace
 - iii. COMMAND + ‘s’ = Save Workspace
 - iv. COMMAND + SHIFT + ‘s’ = Save Workspace As
 - v. Close Current Workspace
 - 1. On Mac = COMMAND + ‘w’
 - 2. On Linux and Windows = CTRL + ‘Q’

- d. Selection

- i. COMMAND + ‘a’ = Select All
 - ii. COMMAND + ‘d’ = Deselect All
 - iii. COMMAND + ‘=’ = Grow Selection
 - iv. COMMAND + ‘-’ = Shrink Selection
 - v. SHIFT + CLICK = Add to Selection
 - vi. SHIFT – CLICK = Remove From Selection

- e. Edit
 - i. COMMAND + 'z' = Undo
 - ii. SHIFT + COMMAND+ 'z' = Redo
 - iii. COMMAND + 'c' = Copy
 - iv. COMMAND + 'x' = Cut
 - v. COMMAND + 'v' = Paste
 - vi. COMMAND + 'b' = Paste Bonded
 - 1. Paste atoms automatically bonded to the one from which they were copied.
- f. View
 - i. SHIFT + COMMAND+ SPACE = Focus on Visible Objects
 - i. COMMAND+ SPACE = Focus on Selected Objects
 - ii. 'h' = Hide Selected Objects
 - iii. Option 'h' = Show Hidden Objects
- g. Camera
 - i. COMMAND+ 'p' = Capture Camera Image
- h. QUICK NAVIGATION MENU
 - i. SPACE