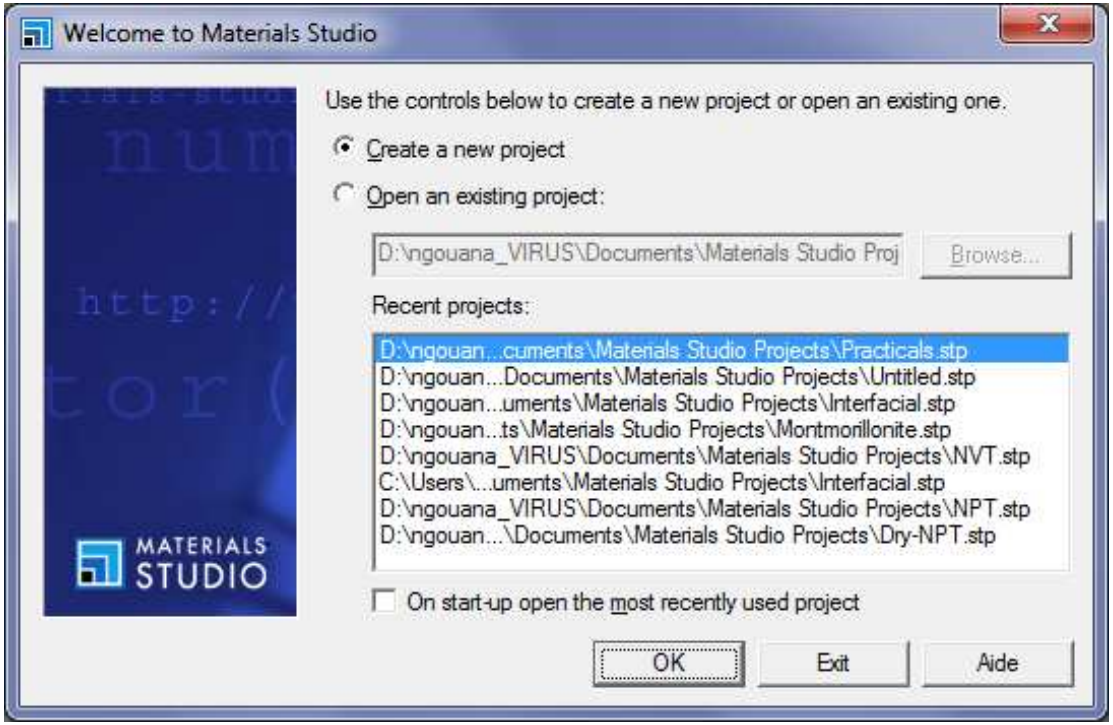
Using Materials Studio to Prepare and Run MD Simulations and Analyze the Results

Outline

- Drawing an organic molecule using the sketch tool.
- Building a crystal structure (kaolinite, pyrophillite, talc, quartz…)
- Cleaving the crystal along a certain crystallographic plane to create a surface
- Optimizing crystal structure (geometry optimization or energy minimization)
- Creating a water box of 64 H_2O molecules and optimizing its structure
- Creating an aqueous solutions of (Na^+, Cl^-), or (Cs^+, Cl^-), (Ca^{2+}, Cl^-) or (Sr^{2+}, Cl^-) … and using them to run MD and analyze the results
- Running MD Simulations
- Analyzing the MD results
- Creating a slab of aqueous solution and adding it on the crystal surface
- Running MD simulations for the interfacial clay-solution system and analyzing the results.

1. Drawing an organic molecule using the sketch tool

- **Open Materials Studio.**
- **Choose '*create a new project*' and name your project.**

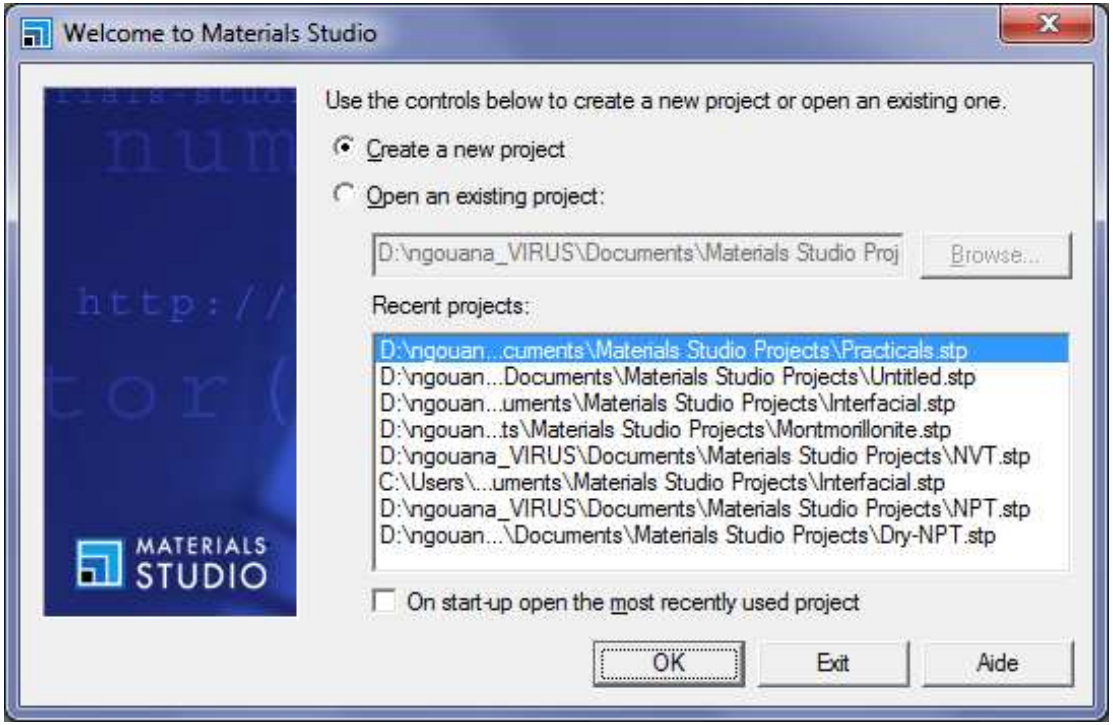


- **Right click on the name of your project -> *New* -> Folder Name it , e.g. '*NOM*'**

- **Now you can start sketching a model molecule of NOM (Natural Organic Matter) using the structure shown in the red frame of the file TNB-NOM-sein-est-1999-p1.pdf.**

2. Creating a new MS project and building a crystal structure

- **Open Materials Studio.**
- **Choose '*create a new project*' and name your project.**



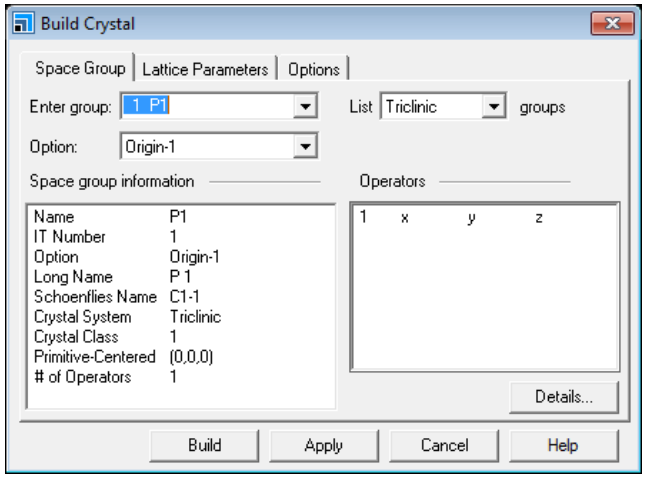
- **Right click on the name of your project -> *New* -> Folder Name it , e.g. '*crystal*'**

- **Now you can start building the crystal or import (load) a template from a library.**

2 (cont.). Building a crystal (kaolinite, pyrophillite, talc, quartz…)

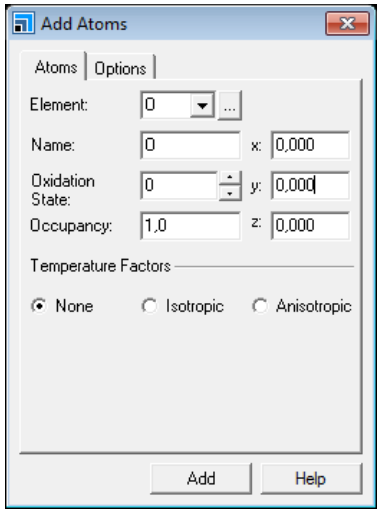
You will be provided with unit cell atomic positions of some crystals. Choose one the structures and build the crystal.

- **Go to Build -> Crystals -> Build Crystal**



Under Space group menu select the lowest symmetry group (P1), ignoring the symmetry group given by the atomic structure file. Then under Lattice Parameters enter the box lengths and angles.

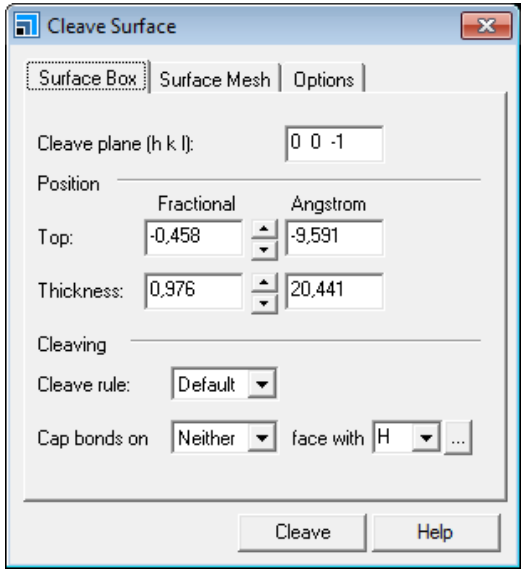
- **Go to Build -> Add atoms**



Input the coordinates for each atom to generate the crystal structure. Use the coordinates provided by the table "Co-ordinates for all atomic positions", but the identity of the atoms/elements (NoP) should be taken from the previous table in the same file.

3. Cleaving the crystal to create a surface

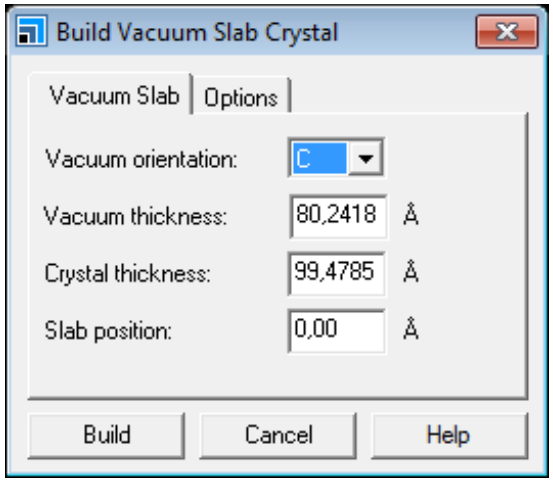
- Go to **Build -> Surfaces -> Cleave Surface**



- **Define the cleavage plane (usually, it is (0 0 1))**
- **Define the thickness of the crystal**

Cleave

- Go to **Build -> Crystal -> Build Vacuum Slab…**



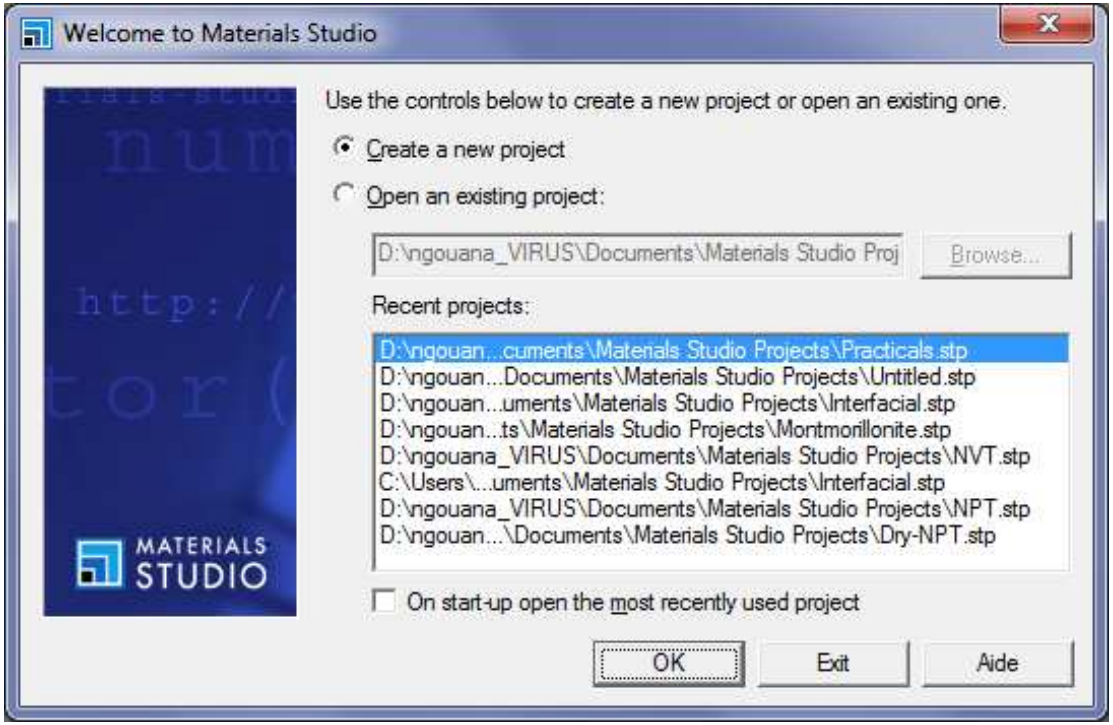
- **Choose the vacuum orientation**
- **Define the vacuum thickness (to be filled with aqueous solution later)**

Build

- **Add hydroxils (OH groups) to the dangling bonds, if necesssary**

4. Creating a water box of 64 H_2O molecules

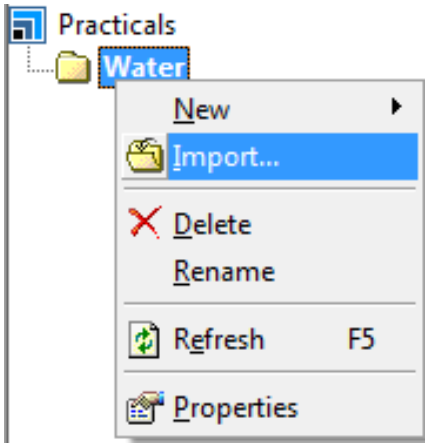
- **Open Materials Studio.**
- **Choose '*create a new project*' and name your project.**



- **Right click on the name of your project -> *New* -> Folder Name it '*Water*'**

- **Now you can import (load) a template or build a model within the water folder.**

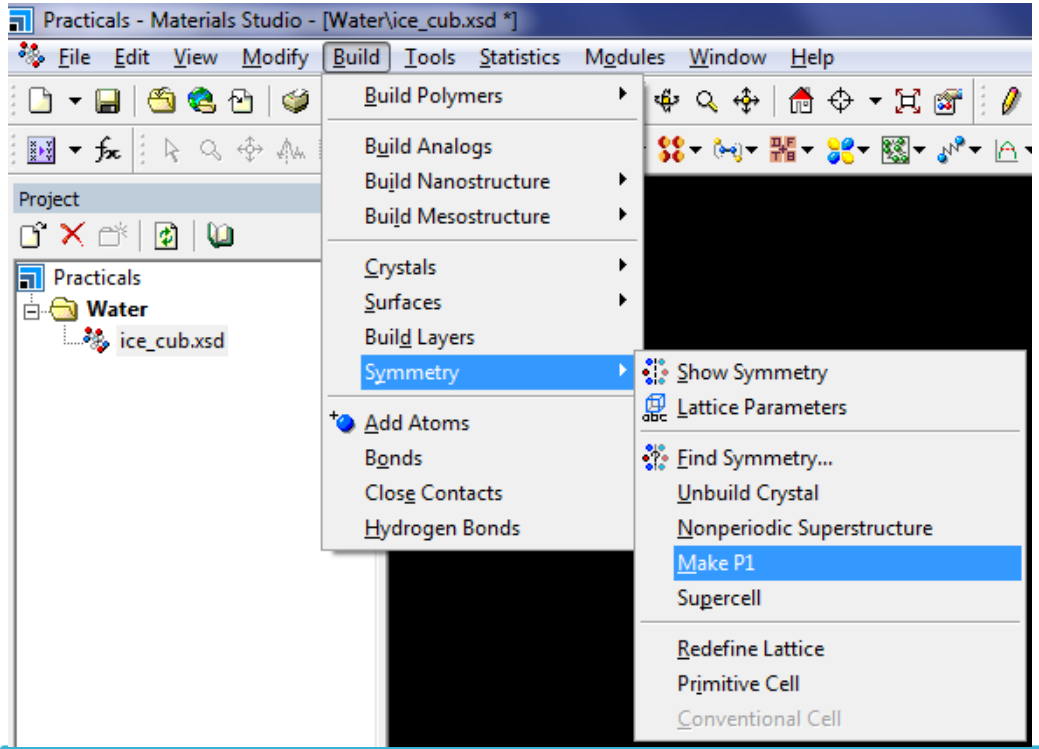
Importing a template from the database



- Right click on the Water folder, then click on Import and go to /Structures/molecular-crystals/misc/ directory

- Chose the cubic ice structure (ice_cub.msi)

- Change space group to P1

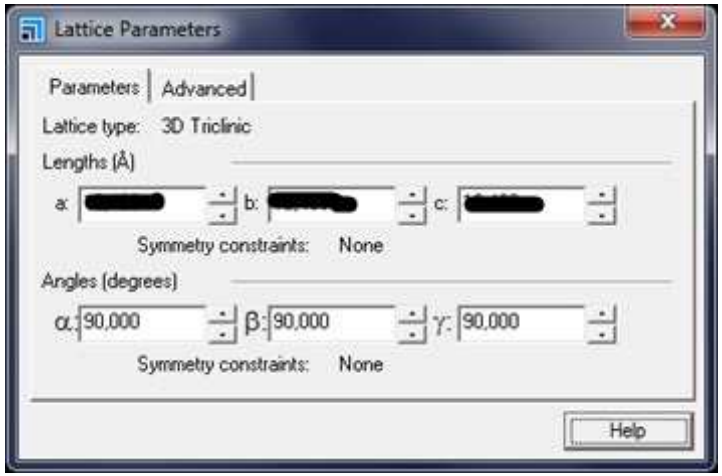


You now have a unit cell with 8 water molecules (go to Edit -> Atom Selection menu to check for this). In order to make a simulation cell of 64 water molecules, you need to multiply the unit cell by (2 x 2 x 2) in the x, y , and z directions.

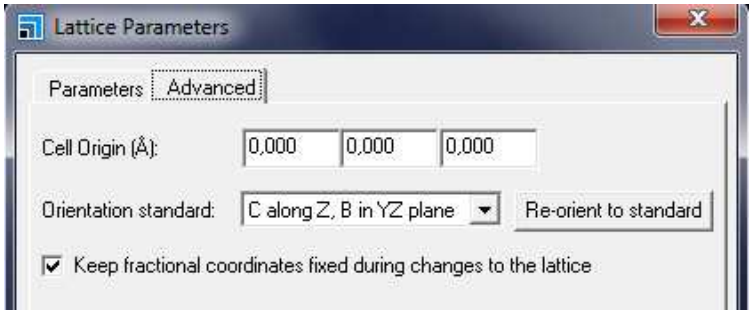
- **Create a supercell:** Build -> Symmetry -> Supercell. Set supercell range to 2 for A, B and C and then click on supercell.

- You need now to resize the supercell dimensions to have them all equal. To do this you must calculate the volume needed to fit 64 water molecules in order to target a density of about 1 g/cm^3. Find out this volume and from it, determine a, b, and c dimensions.

- Then, right click in the dark area -> Lattice Parameters -> Parameters. Now enter the a, b, and c values you just determined above.



- Make sure fractional coordinates are kept fixed while doing this.

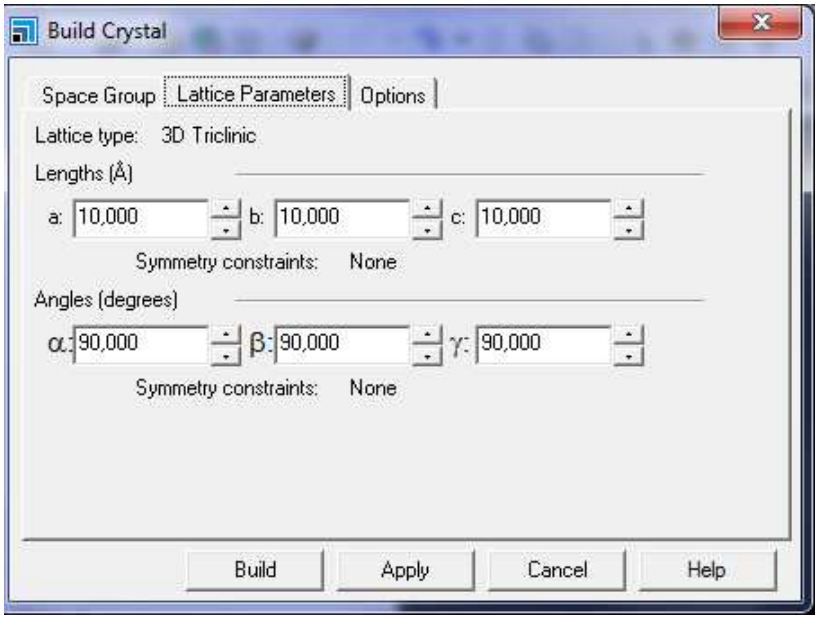


Alternative method of creating a water box

- In the Water folder right click -> New -> 3D Atomistic Document. Rename it to water.xsd.

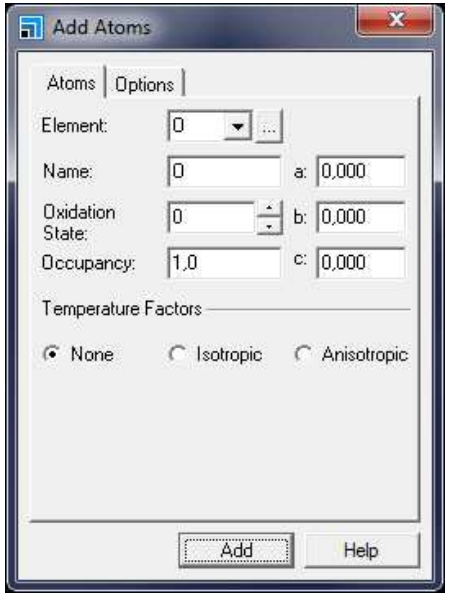
- Build a cubic crystal with a volume corresponding to 1 H_2O molecule: Build -> Crystals -> Build Crystal.

- As you did before, find out the volume needed to fit 1 H2O molecule if the density is equal to 1 g/cm^3. From the volume deduce the box dimensions.



- Select 1 P1 under Space group menu and enter the box dimensions you just determined under the Lattice Parameters menu.

- Then, Build -> Add Atoms -> Atoms.



- Choose Element O and enter the appropriate oxidation state. Set occupancy to 1,0, and atomic positions (a, b, c) so that the O atom is located at the center of the box.

- Click on the created O atom. Then Modify -> H Adjust Hydrogen

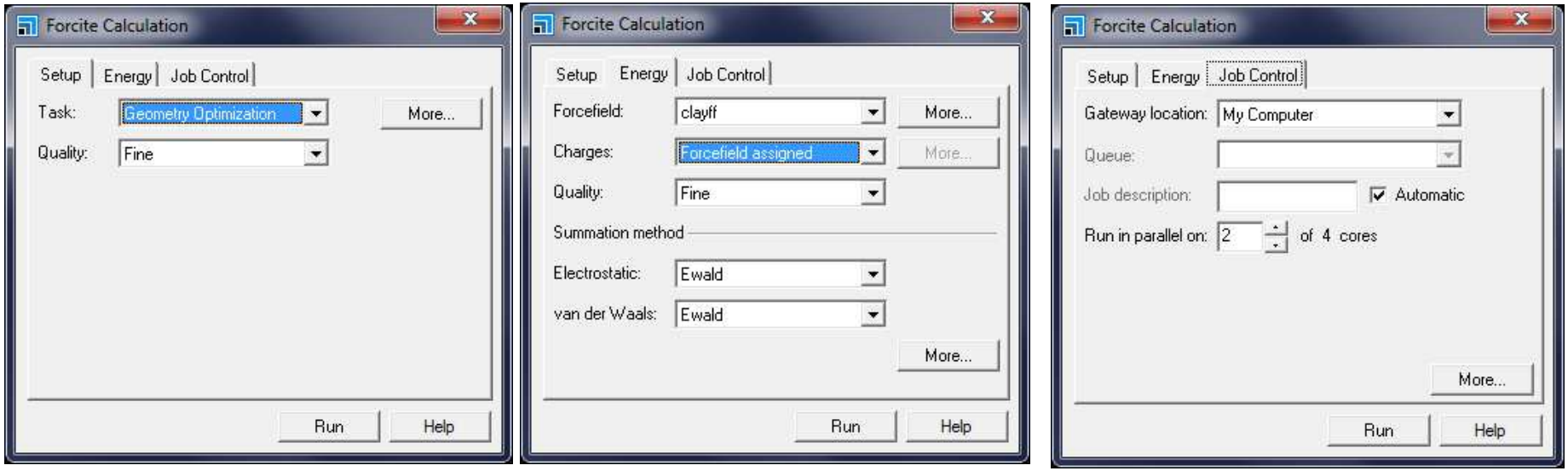
- You now have a box of 1 H_2O molecule.

Transform if into a box of 64 H_2O molecules.

5. Minimizing the crystal energy
(this part can be performed after connection to the license server)

- Go to Module -> Forcite tools. Click on the icon and then select Calculation.

- **Select a task**
- **Select the Forcefield**
- **Set Computer options**



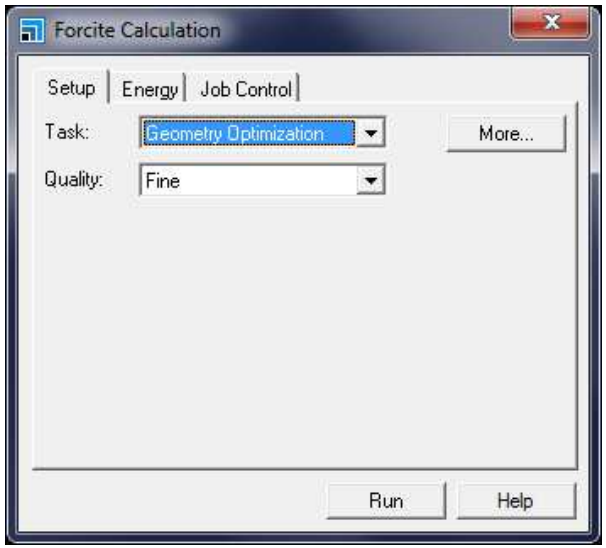
- **Click on More… to set options for the Task (where and if necessary)**

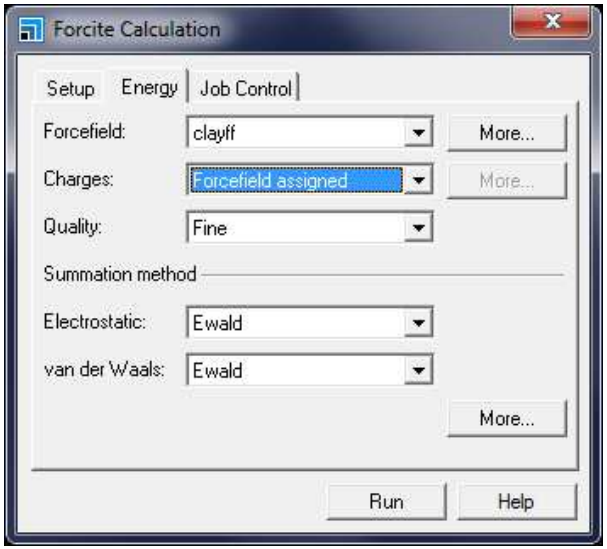
- Run

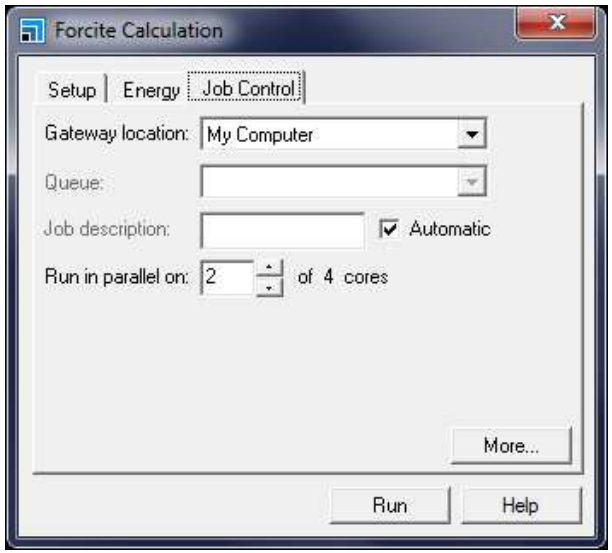
6. Minimizing the energy (while connected to the license server)

- Go to Module -> Forcite tools. Click on the icon and then select Calculation.

- **Choose a task**
- **Choose the Forcefield**
- **Set Computer options**







- **Click on More… to set options for the Task (where and if necessary)**

- Run

7. Creating aqueous solutions out of a pure water simulation box

- Create a new folder and a new 3D Atomistic Document in this folder. Then, open the minimized structure of water and copy paste it in your newly created 3D Atomistic Document.

- Select one O atom. Then go to Modify -> Modify Element -> Periodic Table and choose the element (Cs, Ca, Cl, Na, Li…) you want to replace with. Delete the two H atoms bonded to this new element.

- Repeat the procedure to add more elements of the same types.

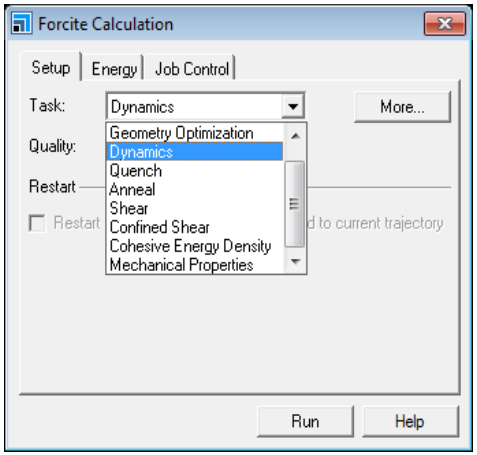
- Remember that the elements you are adding are ions, double check that you have added an equal amount of positive and negative charge by your modifications in order to keep the total system neutral

- Minimize the energy of your system

8. Running MD Simulations (while connected to the license server)

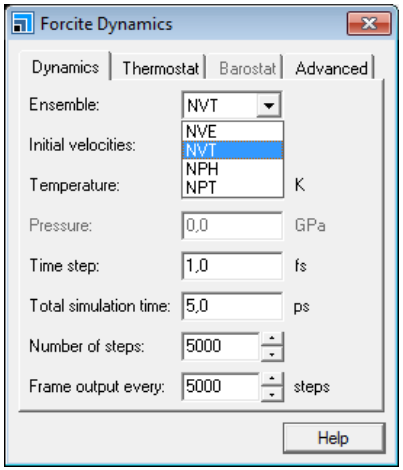
- Go to Module -> Forcite tools. Click on the icon and then select Calculation.

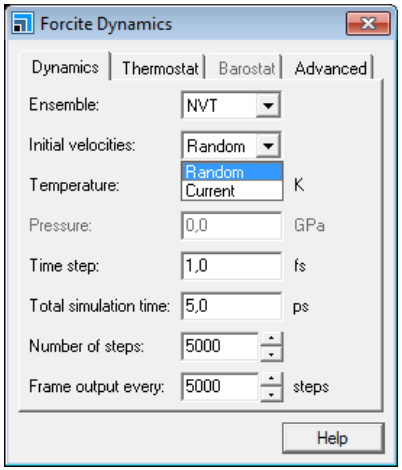
➢ **Choose a task**

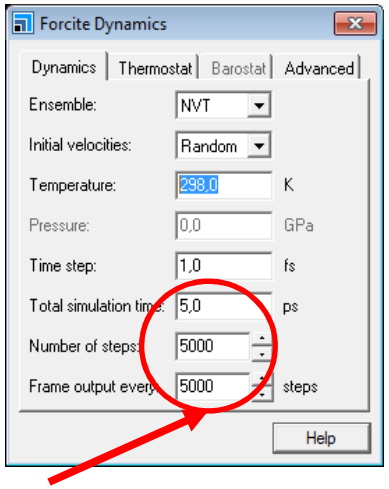


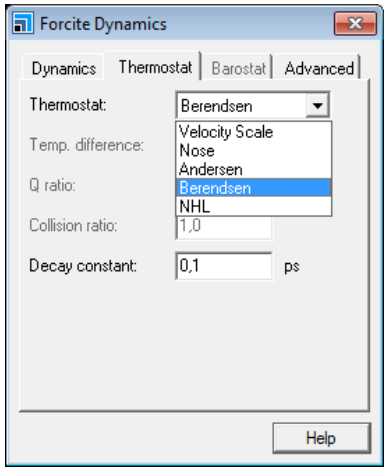
➢ **Click on More… to set options for the Task**

➢ **Choose Ensemble, option for initial velocities, Temperature, Timestep, Thermostat…**



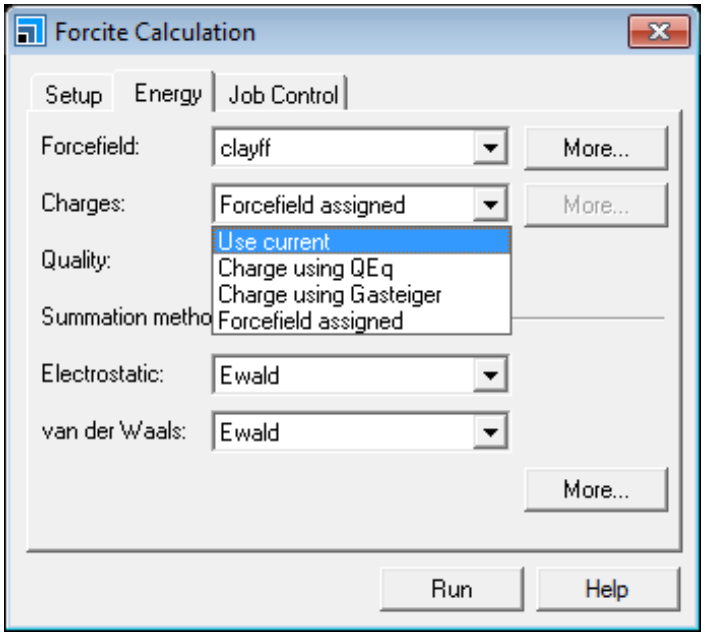


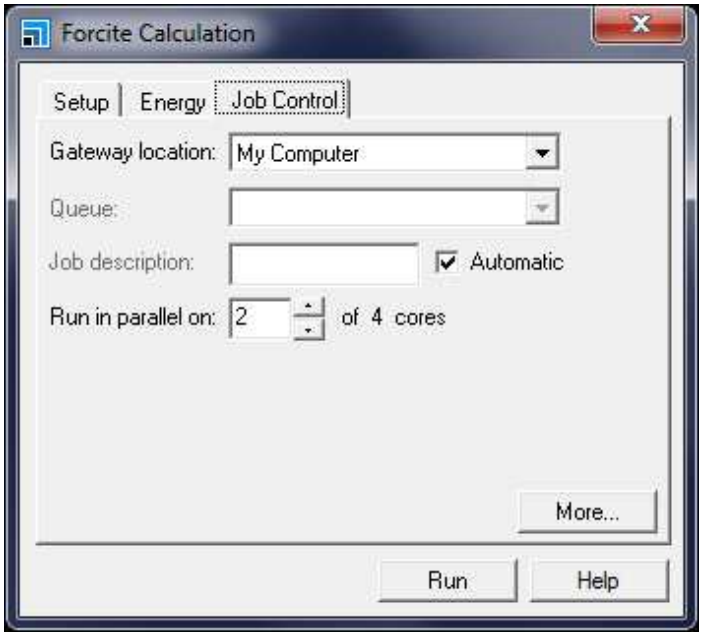




These values can be 30, 30000, 100 for equilibration and 50, 50000, 4 after the restart to accumulate data for your equilibrium trajectory

➢ Choose Forcefield, Set Computer options and Run

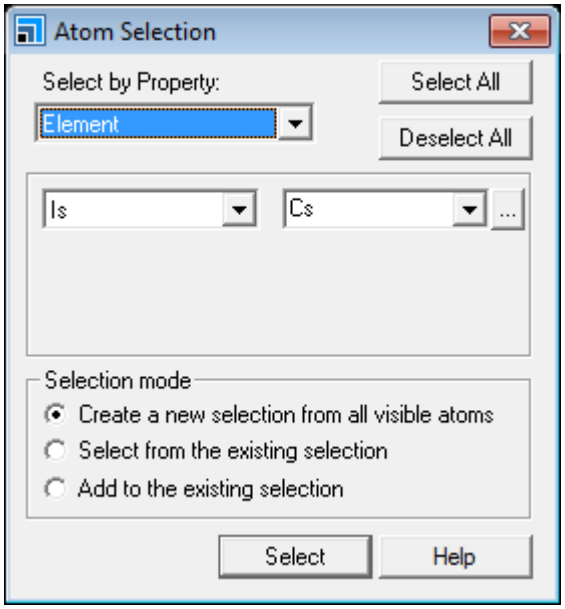




9. Analyzing the results (while connected to the license server)

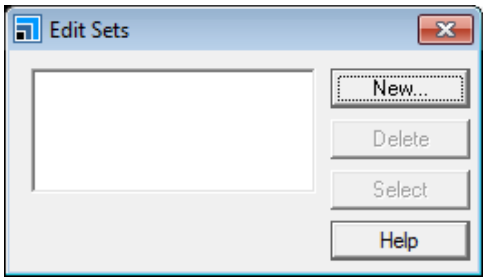
❖ **Before carrying out analysis, you need first to specify different groups of atoms in the system.**

➢ **Go to Edit -> Atom Selection**

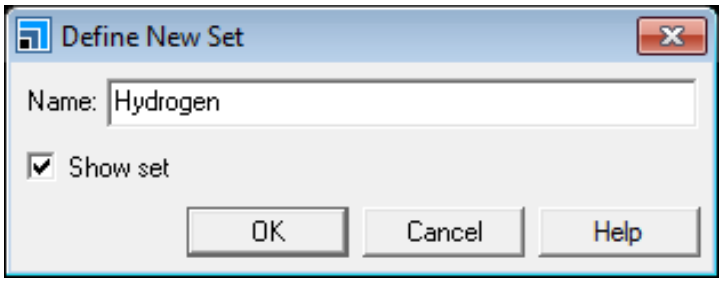


➢ **Select the one atom or a group of atoms that will be used for analysis.**

➢ **Go to Edit -> Edit Sets**



➢ **Click on New and give a name to the set of atoms**



➢ **Repeat the previous steps to define other sets of atoms**

❖ Go to **Module -> Forcite tools**. Click on the icon and then select **Analysis.**

A list of properties is displayed on the left and their type (structural, dynamical, statistical) is given on the right.

Here we are going to look at the following properties:

Statistical properties

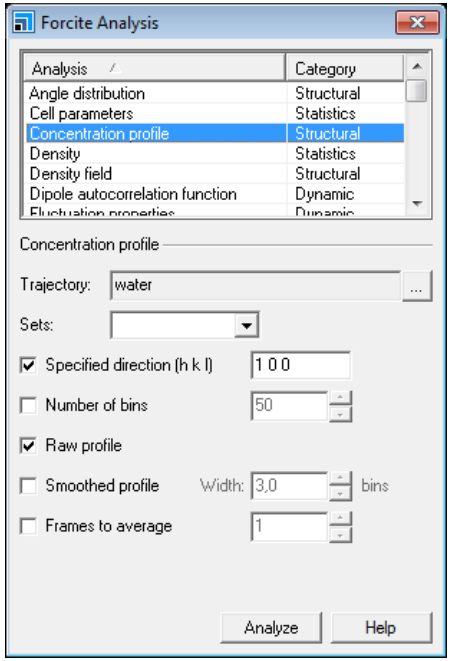
- ✓ **Temperature**
- ✓ **Pressure**
- ✓ **Hamiltonian**
- ✓ **Potential energy components**
- ✓ **Total kinetic energy**

Structural properties

- ✓ **Radial distribution function (max distance – 10A)**
- ✓ **Concentration profile (think about the directions: (0 0 1), (0 1 0), or (1 0 0); increase the number of bins to 500)**

Dynamical properties

- ✓ **Mean squared displacement**
- ✓ **Velocity autocorrelation function and Power spectrum (use 3ps as the maximum length of the VACF calculation)**



- ➢ **Click on the property you want to analyze**
- ➢ **Choose the sets of atoms (some properties require one set, some others – two)**
- ➢ **Choose or insert the appropriate options**
- ➢ **Click on Analyze to launch the analysis**