Calculating heat of fusion of polyethylene using Polymer Modeler at nanoHUB

In this tutorial:

- Setup MD simulations of polyethylene (PE), both amorphous and crystalline configurations
- Determine the heat of fusion of PE

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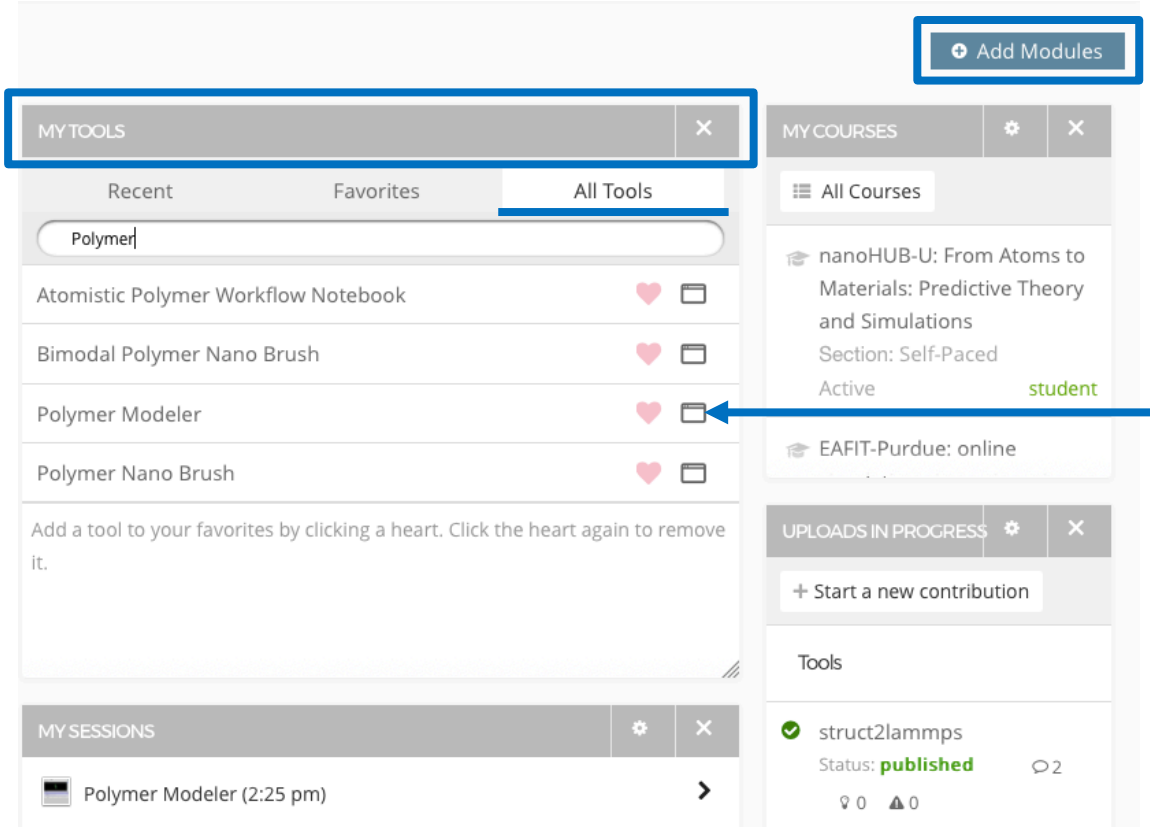
Step 1: Launch Polymer Modeler tool

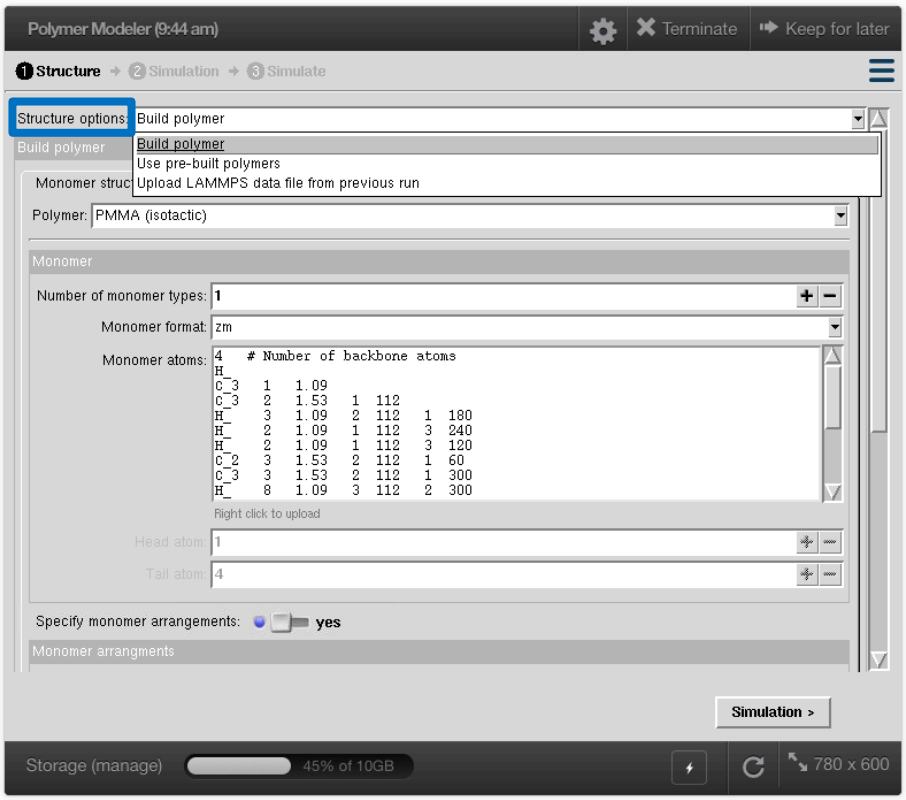
In your nanoHUB dashboard you will see MYTOOLS Module, if not you can get it in the Add Modules box



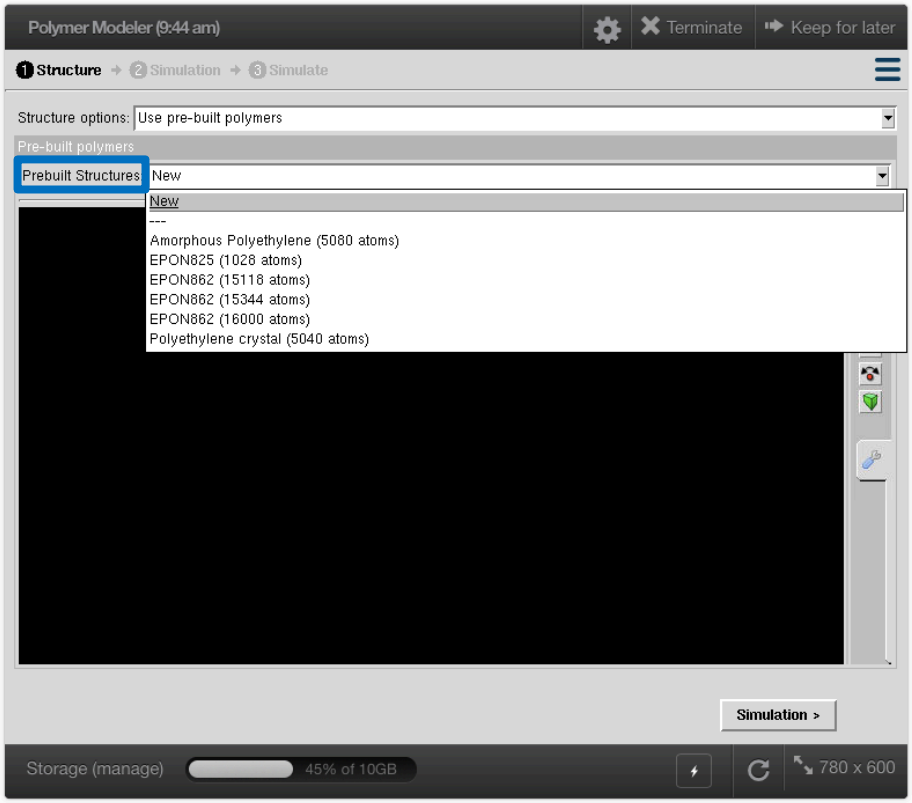
- All tools tab
- Search *Polymer Modeler*
- Launch tool (click in small box)

Step 2: Select the polyethylene structures

- Select **Use pre-built polymers** in the Structure options menu

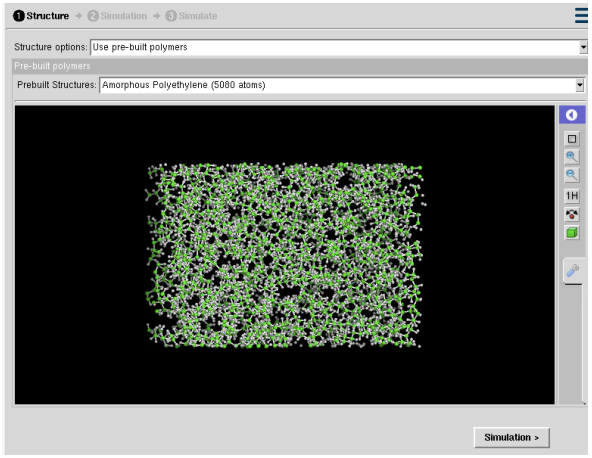


- Select **Polyethylene (amorphous)** in the Prebuilt



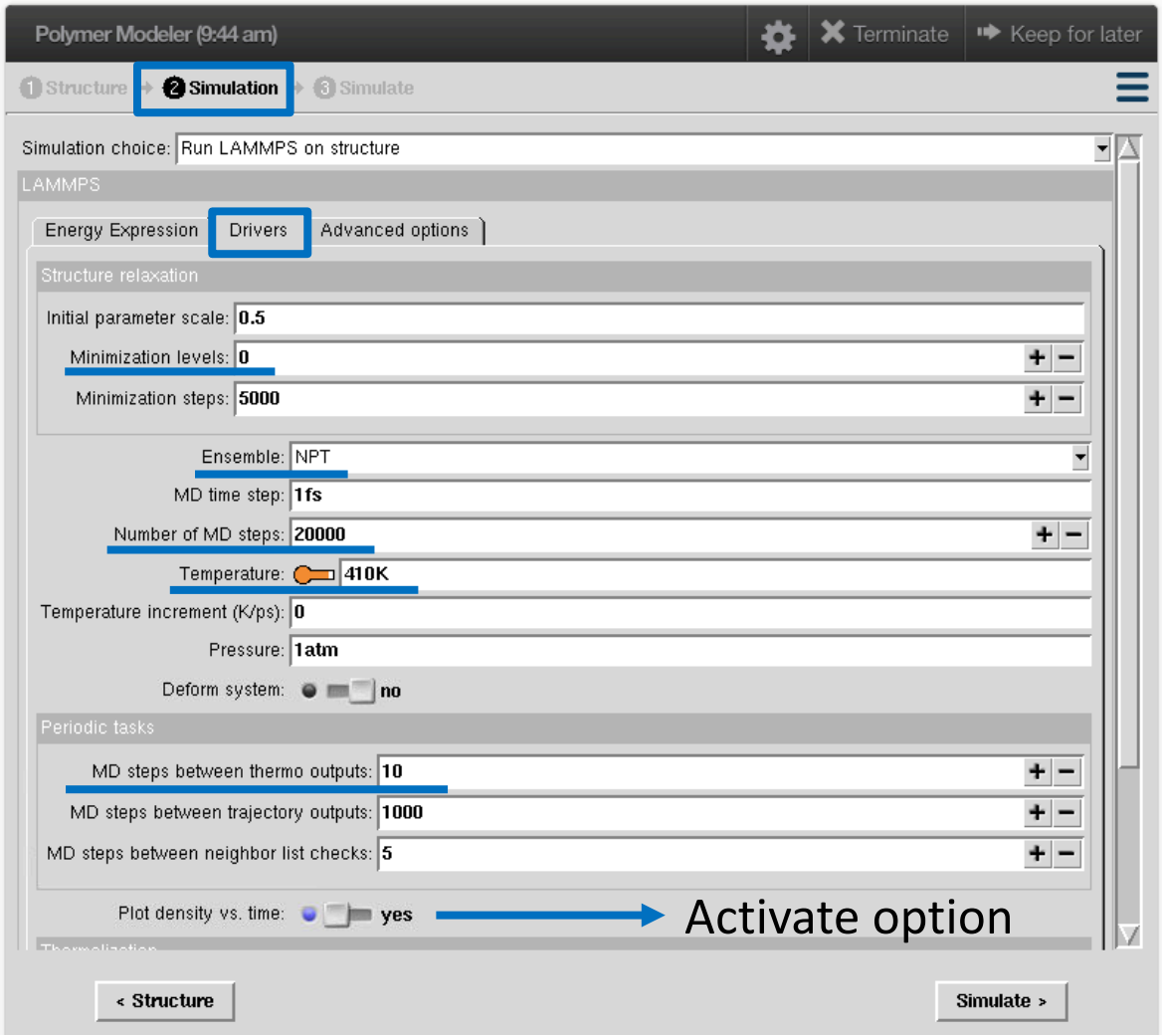
Step 3: Set up the simulation

Once the structure is selected you can visualize it

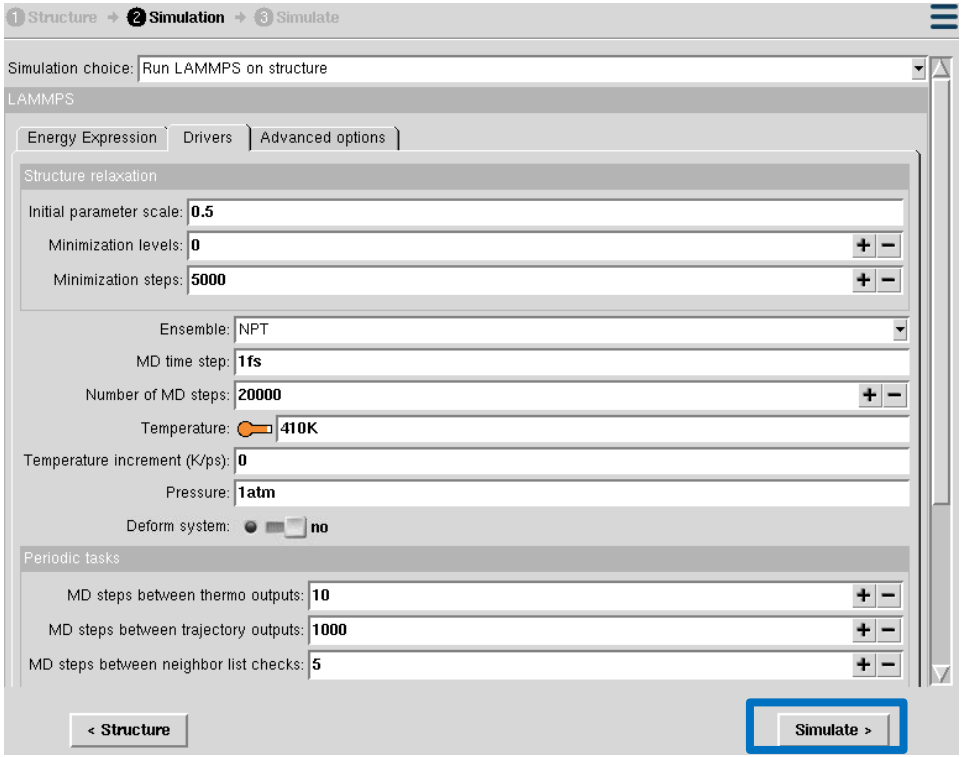


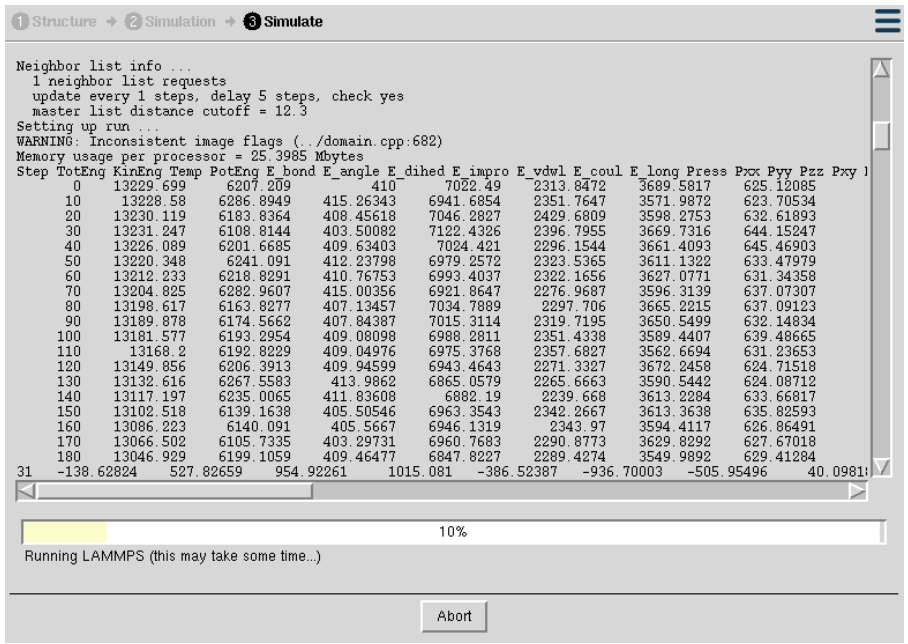
- Change **Minimization levels** to zero
- Change **Ensemble** to NPT
- Increase **Number of MD steps** to 20000 (20 ps)
- Change **Temperature** to 410K

- Select **Simulation** tab and **Drivers** menu



Step 4: Click simulate, wait for results



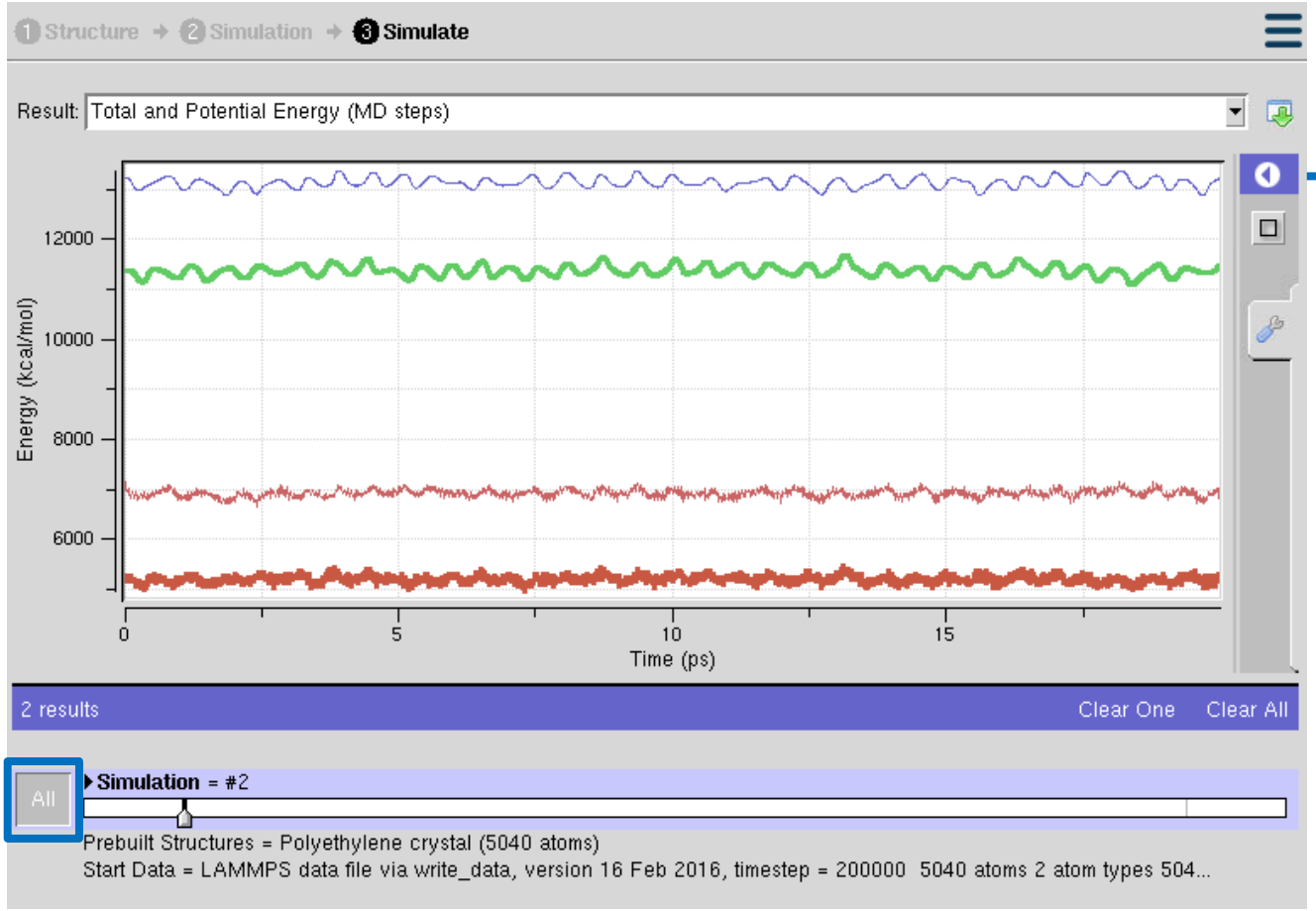


Step 5: Once it finishes, repeat same procedure for prebuilt Crystal Polyethylene

Just go back to the **Structure tab**, no need to open a new Polymer Modeler

Step 6: Analyze data

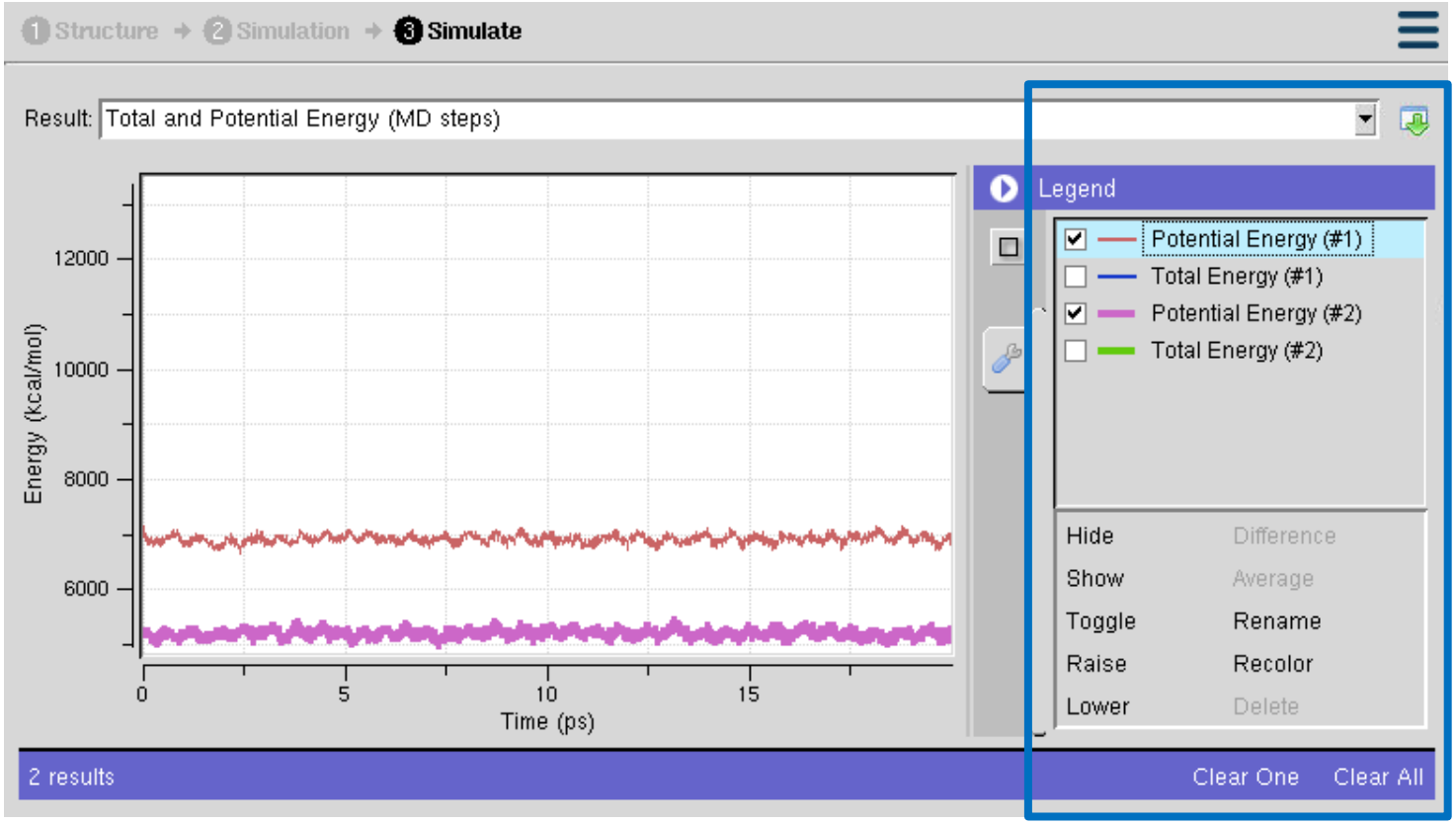
- Select result: **Total and Potential Energy**



- Click **here** to recolor and rename data
- We will also unselect the Total Energy output

- Click **All** and you can visualize both results in the same screen

Step 6: Analyze data (Continuation)



- Once unselect the Total Energy output
- Click in the download bottom (right corner) and save file. It will contain the time and Potential Energy for each simulation case in order of simulation, for this case #1 is Amorphous PE and #2 Crystal PE

Step 7: Calculate heat of fusion

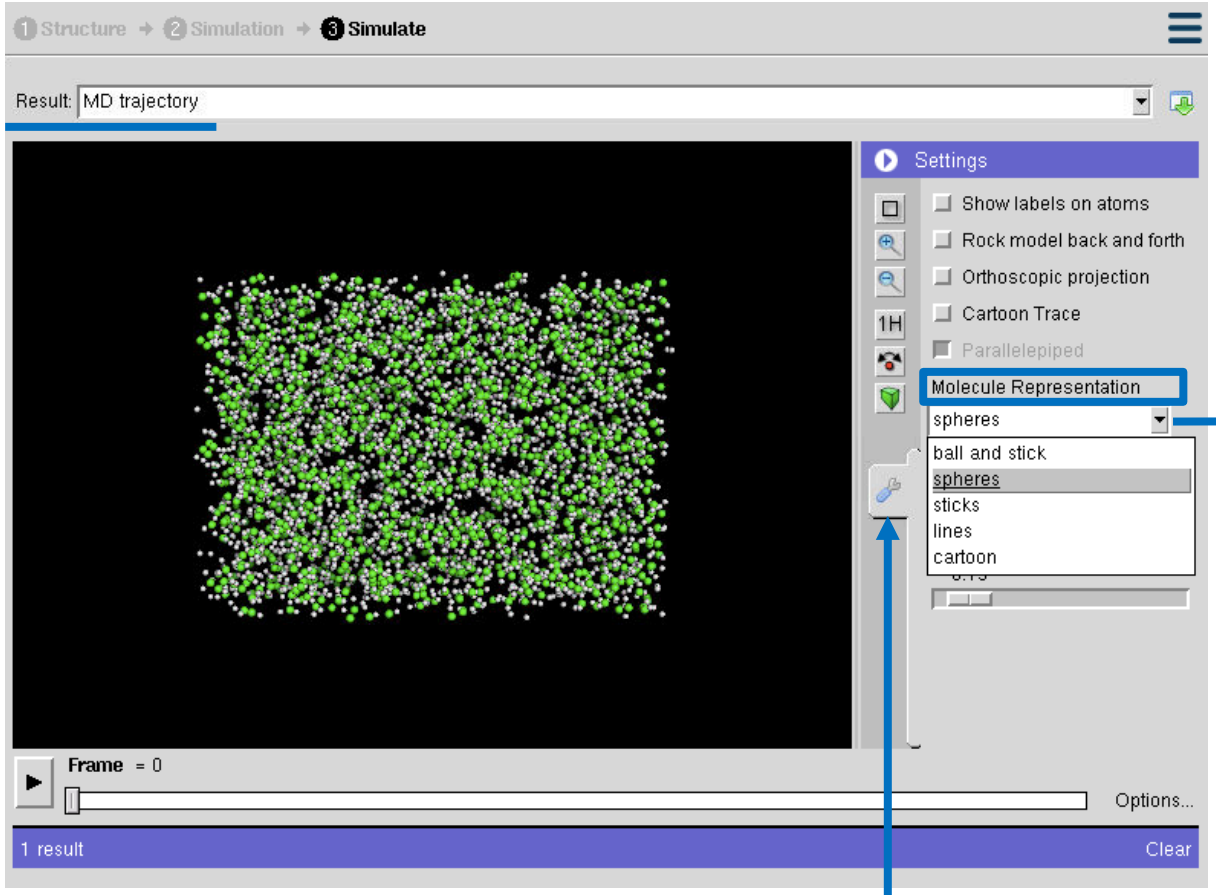
- Get an average of the Potential Energy for each simulation (you can import the data to Excel for example)
- Parameters of interest:
  - Number of Monomers in simulated PE = 840
  - Molecular weight monomer ($\mathrm{MW_m}$) = 28 g/mol
  - Conversion 1 Kcal/mol = 4.184 KJ/mol

$$\langle \mathrm{d}H \rangle = \left(\frac{\langle PE(\mathrm{Amorphous}) \rangle - \langle PE(\mathrm{Crystal}) \rangle}{\mathrm{Monomers}} \right) * \frac{1}{\mathrm{MW_m}} \text{ [Kcal/g]}$$

$$\langle \mathrm{d}H \rangle = \langle \mathrm{d}H \rangle \text{ [Kcal/g]} \times 4.184 \times 1000 \text{ [J/g]}$$

MD trajectory visualization

- To visualize the MD trajectory select this option in the Result menu



2. Change Molecule Representation to spheres

1. Open the Settings option clicking here

Heat of fusion (example)

- We have obtained the averaged potential energies for a simulation of crystal PE:

$$\langle PE(\text{Crystal})\rangle = 5205.6 \pm 72.6 \text{ [Kcal/g]}$$

$$\langle \mathrm{d}H\rangle = \left(\frac{\langle PE(\text{Amorphous})\rangle - [5205.6 \pm 72.6]}{840}\right) * \frac{1}{28} \text{ [Kcal/g]}$$

$$\langle \mathrm{d}H\rangle = [X \pm \text{error}] \text{ [Kcal/g]}$$

$$\langle \mathrm{d}H\rangle = [X \pm \text{error}] \times 4.184 \times 1000 \text{ [J/g]}$$