# Classroom Challenge: Design Your Own Water Model

Water is the most important molecule in biochemistry. Yet in molecular simulations, we cannot represent it with all its quantum complexity — we need to simplify it into a classical “model” that computers can handle.  
  
That is: a computer program simulating the motions of water molecules must be given an idea about what each water molecule looks like, what interactions to calculate, and the quantities needed to calculate those interactions.  
  
Today, your group’s challenge is to invent your own water model: a simplified representation of a water molecule for simulations. You’ll need to decide:

* How many interaction sites (atoms or dummy points) will it have?
* Where do you place charges?
* Do you include Lennard–Jones (LJ) interactions, and on which sites?
* Will you aim for speed (simpler, fewer sites) or for accuracy (more parameters, more realistic)?

At the end, you’ll present your model, explain your reasoning, and we’ll compare it to real models scientists use (SPC, TIP3P, TIP4P, TIP5P).

## A circle with a number of mathematical equations AI-generated content may be incorrect.Example: A “Too Simple” Water Model

Imagine we try to make water as simple as possible:

* Geometry: A sphere of radius 1.5Å.
* Charges: One negative charge at the center.

This is essentially a (bad) 1-site water model.  
  
**Benefit:**  
- Extremely fast to simulate (only one particle per water molecule).  
**Drawbacks:**  
- Completely unrealistic: the net charge on each water molecule means mutual repulsion between all water molecules. The lack of hydrogen atoms also means no hydrogen bonding, no dipole moment, and no correct liquid structure.

## Your Task

1. Sketch your water model. Decide e.g. how many sites, where charges go, potentials and values like force constants

2. Justify your choices. Why this geometry? Why these charges?

3. Think about tradeoffs. Is your model fast but inaccurate, or slower but more realistic?

## Presentation

You will be asked to sketch your water model on the blackboard, as will one other group. You will then highlight a difference between these 2 models, and some implication of that difference. You may also be asked to elaborate further on some aspect of your model.