

Table 1: Summary of parameters

Parameter	Mumerical
Number of particles	150-300
Number of iterations	2
Temperature (°C)	-24 ~ -22
Temperature (°C)	-30 ~ -28
Time (ns)	5-8
Time / step (ns)	1.5
Time step (fs)	20P
Time step (fs)	17.13
Time step (fs)	5.914
Time step (fs)	8.75
Time step (fs) (L)	300
Time step (fs)	10803 × 2020 × 2731

Simulation box

Simulation box:

The simulation box is a rectangular prism with dimensions 10803 Å × 2020 Å × 2731 Å. The box contains a water molecule and a chocolate molecule. The water molecule is represented by three oxygen atoms (red) and two hydrogen atoms (white). The chocolate molecule is represented by a complex structure of carbon (grey), oxygen (red), and hydrogen (white) atoms. The simulation box is centered in the middle of the simulation cell.

: Simulation box & simulation parameters
 The simulation box is a rectangular prism with dimensions 10803 Å × 2020 Å × 2731 Å.
 The simulation parameters are as follows:

Simulation box:

1. Simulation box dimensions: 10803 Å × 2020 Å × 2731 Å.

Simulation box dimensions: 10803 Å × 2020 Å × 2731 Å.

Simulation box:



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