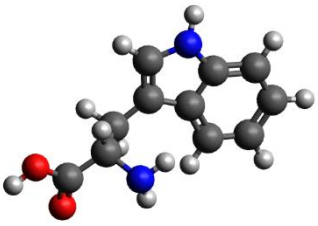
Activity - Molecular Dynamics Simulations



How can we understand what is happening at an atomic or molecular scale?

With computers, of course! In the 1950s, researchers developed methods to study atomic systems by representing each atom as a rigid sphere. However these had many challenges and could not be applied to complex, real-life systems since computers had limited power and capacity and suitable algorithms had to be developed. Since digital computers have been made available and more powerful over the last decades, the number of simulation techniques has greatly expanded and using complex computational methods to look at atomic systems has become a very useful tool.

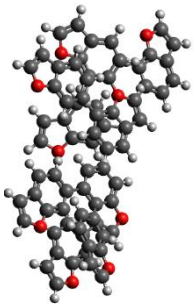
So how exactly does a computational model mimic what atoms do in real life?

Let's take a look at one popular method: molecular dynamics simulations.

Molecular – molecules are made up of atoms connected by chemical bonds

Dynamics – dynamics is the study of forces and how they affect motion

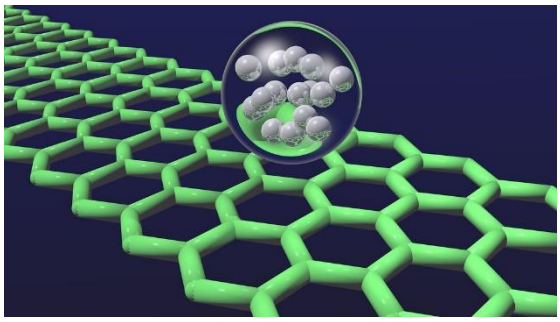
Simulation – a simulation is an imitation of a real process, in this case on the computer



Molecular dynamics is a computer simulation method used to study the behaviour of atoms and molecules. Everything moves because of forces, which result from the interactions among atoms and molecules. Molecular dynamics involves evaluating the physical movement of atoms in order to observe the evolution of a system over time and provide insight into system properties.

How do we describe the physical movement of atoms?

Molecular dynamics simulations use the classical equation of motion, also known as Newton's second law (force = mass x acceleration), to determine the time-dependent positions and velocities of atoms within a system. In other words, molecular dynamics works to numerically solve an N-body problem of classical mechanics.



Here is an overview of how it works:

First, the user must provide initial conditions to the simulation. This includes a list of all the atoms in the system and their initial positions (usually given in Cartesian format as a list of x, y, and z coordinates), as well as system information such as temperature and pressure.

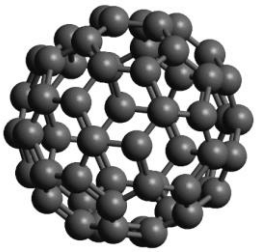
Then the molecular dynamics code calculates forces between bonded and non-bonded atoms based on the energy functions (also known as a force field) within the simulation. For example, the force between two bonded atoms is often modelled through a harmonic potential (think: spring equation) based on the distance between the two atoms. Non-bonded atoms interact with each other through van der Waals forces and electrostatic forces. These forces are then integrated once to get the atomic momenta and twice to calculate the new atomic positions caused by the forces acting on the atoms, since we also know that force, F, is equal to the negative derivative of the energy, U, with respect to the distance between the atoms, r. That is, $F = -dU/dr$.

Then the simulation recalculates the forces between all of the atoms in their new positions and double integration again gives an updated list of atomic coordinates. These steps are repeated

a large number of times, and continue until the desired simulation length is reached or until all the computer time available is used up.

Repeating these energy and force calculations several thousand (or trillion!) times produces atomic trajectories – that is, the x, y, and z coordinates of all the atoms over time.

Molecular dynamics simulations generate information at the microscopic level, namely atom positions and velocities over time. In order to understand materials in a way that can be better applied, this microscopic information needs to be converted to macroscopic quantities that can be measured experimentally, such as pressure and temperature. To do this, we use statistical mechanics, which uses statistical methods to mathematically relate the desired macroscopic properties to the distribution and motion of atoms/molecules in a system.



In summary:

Input: Atoms and positions, force field parameters, and other system information (such as temperature and pressure)

Simulation: F = m x a = $(-dU)/dr$ → repeat many, many times

Analysis: Distribution and motion of atoms gives macroscopic measurable properties

Molecular dynamics is popular tool that is used in many fields including chemistry, physics, biology, material science, and engineering!

Here are some videos showing the results of molecular dynamics simulations:

- Salt water droplet: https://youtu.be/-cskciZf8oM?t=7
- Bacterial cytoplasm: https://www.youtube.com/watch?v=5JcFqj2gHx8&t=163s
- Protein folding: https://www.youtube.com/watch?v=SMNlfNJKdRc