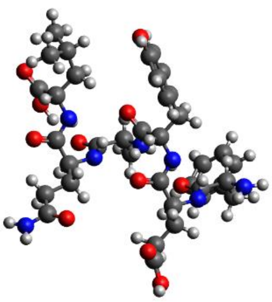
Activity - Applications of Molecular Dynamics

Molecular dynamics is an important tool because it allows us to examine systems at conditions (temperature, pressure, etc.) that may not be feasible in a hands-on experiment. This is important for testing substances within very specific applications, like the material designed for use in a space craft that will be exposed to temperatures, pressure, and radiation not found here on Earth.

Running molecular simulations also allows for much cheaper and faster experimentation than can be done in a non-virtual way. One key example is in designing drugs to treat diseases. Drug development is a very long and expensive process, often taking decades and costing hundreds of millions (or even billions) of pounds. Molecular dynamics simulations are a crucial step that allows scientists and engineers to select the best drug candidates from an initial sample of tens of thousands of compounds. Using fundamental chemical and physical knowledge about these systems, computer experiments can be designed that simulate molecules that have not yet been created in real life and evaluate how well they would do in a specific environment. This is called high-throughput screening because current simulation methods allow thousands of systems to be studied in a short period of time. This is far beyond what can be done experimentally in a laboratory and is a key step to reduce the amount of time and effort is required to produce a final product!

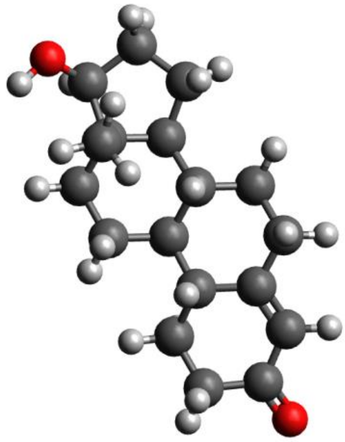


Thinking beyond classical molecular dynamics

What about reactions?

Classical molecular dynamics simulations are not able to model bond breaking or forming between atoms, and therefore fail to simulate chemical reactions. Obviously, this greatly limits the systems that can be studied.

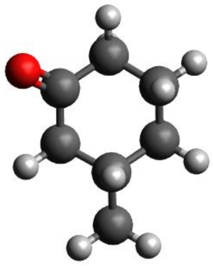
But guess what? In 2001, some smart researchers at the California Institute of Technology developed a reactive molecular dynamics simulation method, called ReaxFF, to deal with this[1]! Note that are several other reactive molecular dynamics simulation methods and many, many more non-reactive ones.



ReaxFF uses the concept of bond orders to describe the energy between atoms in a system. The interatomic distances are used to calculate bond orders, which are then used in all of the energy terms (bonded and non-bonded). This means that the system is not provided with fixed bonds or reactive pathways, but these are calculated within the simulation.

What about quantum effects?

If you've been thinking hard, you may wonder about quantum effects. We know that an atom is made up of a nucleus and electrons that move around it. The electrons move much faster than the nucleus. It becomes clear that at the molecular / atomic scale, the quantum mechanical motion of subatomic components such as electrons can become important! In these cases, we cannot simply use classical Newtonian mechanics to model our system.



This can be done using ab initio (quantum) molecular dynamics, which is based on quantum equations instead of Newton's equations of motion. This gives very accurate results but takes a lot of computer resources to run.

1. Van Duin, Adri CT, Siddharth Dasgupta, Francois Lorant, and William A. Goddard. "ReaxFF: a reactive force field for hydrocarbons." *The Journal of Physical Chemistry A* 105, no. 41 (2001): 9396-9409.