

# TELS PERSPECTIVES

## Nano-Engineering with the Molecular Workbench

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### Overview

This document shows some of the ways that the Molecular Workbench (MW) system can be used to model nano-engineering concepts. MW is a molecular dynamics package developed for education that has been extended in several significant ways to give it broader applicability.

Molecular dynamics uses classical mechanics to predict the motion of particles that act under forces that approximate the forces on atoms and molecules. The basic force used in these simulations is derived from the Lennard-Jones potential, a two-parameter generalized force. One parameter controls the short-range repulsion, representing the interaction of electron orbitals as they begin to overlap. This determines the size of the circle used to represent an atom. The other parameter controls the strength of the long-range attraction, the van der Waals force. Thermodynamics is the most obvious consequence of this force law; all objects are in motion and exhibit the interplay of potential energy due to the forces with the kinetic energy due to motion. The sum of all these energies is the total energy, which must be constant in a closed system and therefore represents a sensitive indicator of the accuracy of the calculations.

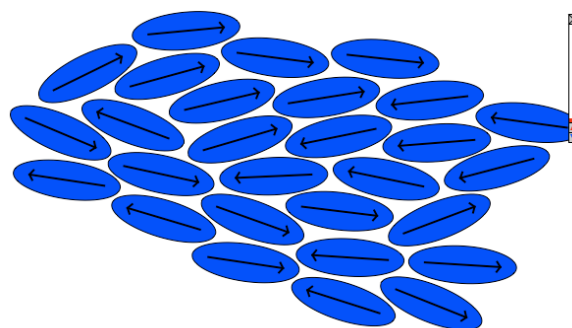
We have added three objects and related forces to the basic molecular dynamics model that allow the system to illustrate some important nano-engineering concepts: Gay-Berne particles, Smart Surfaces, and water interactions.

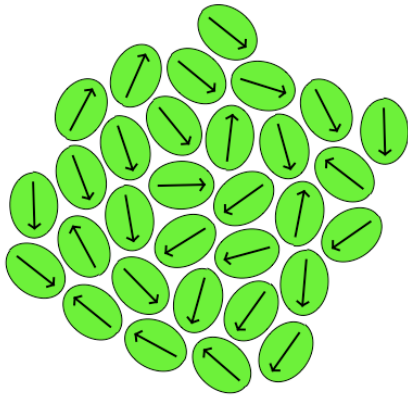
### Gay-Berne Particles

A Gay-Berne particle is an approximation of a large molecule, such as found in liquid crystals, biological systems, and nano-engineering. These particles can be ellipsoidal generalizations of the atoms more commonly used in molecular dynamics. The two parameters of the Lennard-Jones potential are replaced by four parameters that control the size and attractive forces along two orthogonal axes. In addition, these particles can have charge and dipole moments.

The following set of pictures from MW shows nano-particles that self-attract and have dipole moments. These Gay-Berne particles are good approximations of liquid crystal molecules. If they have a chance to move around, without a field, they sometime randomly line up in almost-regular arrays.

If you look closely at the snapshot at right, you can see some of the regularity of a crystal but the lack of long-range order that is typical of a liquid. Running the MW model allows the user to see how the molecules vibrate and randomly slide over on another like so many fish. Note also that the dipole moments, indicated by arrows, are somewhat random, but there is





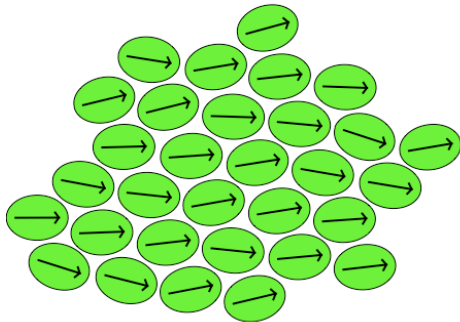
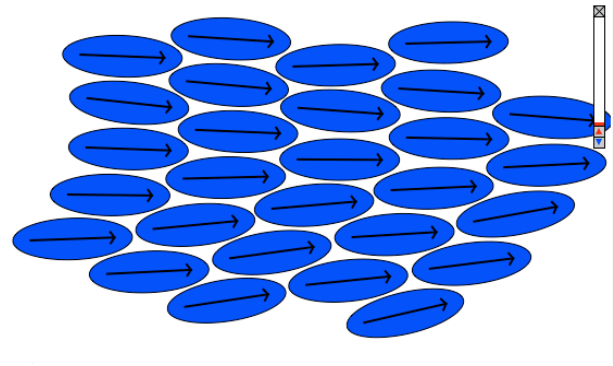
some head-to-tail regularity.

The regularity depends on the shape and dipole moments. The green particles at left are less ellipsoidal and condense into a liquid with much less long-range order, as illustrated.

Turning on an electric field and setting the temperature sufficiently high allows all the dipoles to line up as shown in the illustration at below. Again, the molecules are fairly ordered, but able to slip by one another.

Turning  
on a field

more easily aligns the almost-spherical green molecules, and shown below. Note also, that the field tends to make them more regular, much like a crystal. The same effect can be seen less clearly in the case of the blue particles.

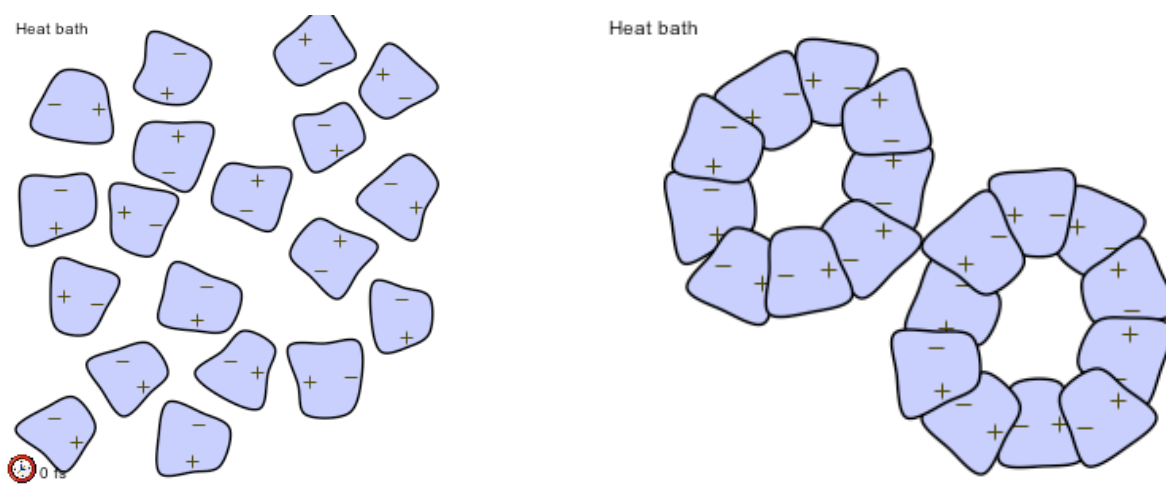


To create your own Gay-Berne models, you can start at <http://molo.concord.org/database/activities/171.html>

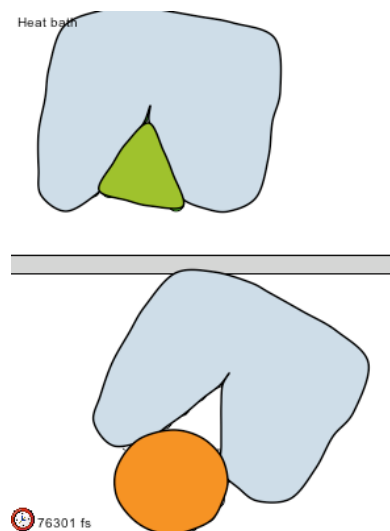
## Self Assembly

Self-assembly is a nano-engineering concept borrowed from biological systems. The underlying mechanism for self-assembly are the general van der Waals mutual attraction of all atoms, Coulomb forces due to charged regions of molecules, and shape. To build in the impact of shape, MW has "Smart Surfaces" that can be drawn by the user. These surfaces are actually chains of MW atoms linked together with elastic bonds and covered by a flexible surface that hides the atoms. Charge can be added to the periphery of a Smart Surface. The result is a good approximation to a large molecule. It can hold its general shape, but it does vibrate, respond to temperature, and have both long-range Coulomb forces as well as short-range van der Waals forces.

Smart Surfaces can be made to self-assemble. Below is an example of a particularly interesting kind of self-assembling object based on nine identical sub-units.



To run this model, launch MW from <http://molo.concord.org/software> and then look for "self assembly" under "Recent models and activities".



The model at the left demonstrates the importance of shape in docking, something similar to self-assembly. This model can be heated to separate the two molecules and then both the ball and triangle bounce around. On cooling, the triangle eventually finds its way back to the complementary surface through a random walk that takes quite a long time. This gives one an appreciation for the time-scale of molecular events of this type.

## Water Interactions and Protein Folding

Another nano-engineering concept modeled with MW is protein folding. The picture below shows a model that illustrates this concept. MW uses a pseudo-field to approximate the effect of hydrophobic forces, which are closely related to surface tension. It requires energy to create new surface area in water, and hydrophobic molecules, in effect, create new surfaces. Therefore there is an energy reduction in moving the molecules to minimize the area of hydrophobic molecules, and whenever motion can result in energy change, there is a force. We apply the force directly because we cannot model all the water molecules that would be needed to produce this force. The resulting protein conformations are not accurate, but they capture the primary ideas.



The chain of balls represents a protein with each ball a different amino acid. The user can change the amino acids and the protein can be placed in water, oil, or a vacuum. When the model is run with water selected, the hydrophilic residues clump in the center and the hydrophobic residues are more likely to be on the periphery. Simulate the effect of a mutation in the DNA that codes for this protein by changing one amino acid, and it is clear that the conformation can change radically, depending on where the change occurs in the protein and whether the charge and hydrophobicity are changed.

This model can be explored by launching the model at <http://molo.concord.org/database/activities/225.html>