Molecular modeling

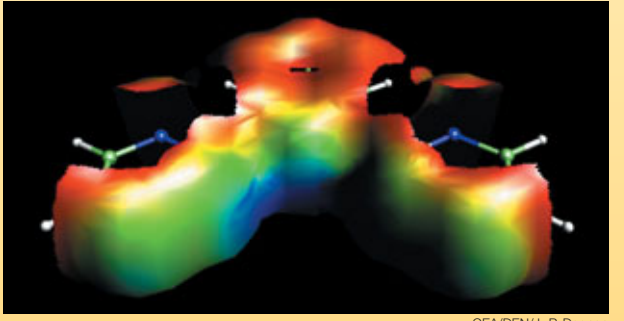
Researchers in biology, chemistry and the physics of materials increasingly use computational tools that enable them to model the behavior of molecules as a function of their structure. The accuracy of these approaches is now such that they are employed for the design of molecules and materials with specific properties.

A broad range of **theoretical** tools is available, including those based on the methods of quantum chemistry, grounded molecular mechanics and molecular dynamics.

Quantum chemistry is grounded on the laws of quantum mechanics and serves, above all, to describe the electronic structure of molecules. This is important for the understanding of processes such as chemical reactions.

Classical **molecular dynamics** simulates the motions of atoms in molecular systems, and the evolution of their spatial configuration, using the equations of classical mechanics. It gives access to structural, dynamic and thermodynamic properties.

Like quantum chemistry, **molecular mechanics** is a method that enables the investigation of the structure and behavior of molecules but it is less costly, faster and can be used to describe systems consisting of thousands of atoms, such as **biological macromolecules**.



CEA/DEN/J.-P. Dognon

Representation of the electrostatic potential around the molecule, bis-triazinyl-pyridine (BTP) calculated by a quantum-chemical method. This molecule was developed for the Sanex process that separates actinides and lanthanides.