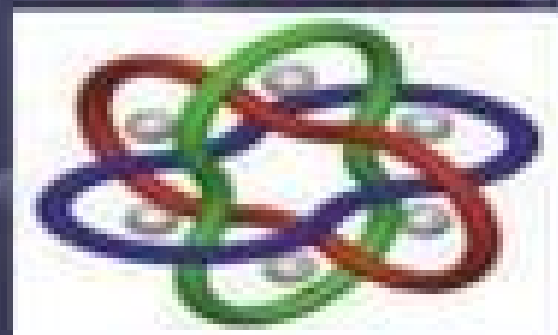


● Molecular mechanics:

- ✓ The "mechanical" model developed to describe molecular structures and properties in as practical manner as possible
- ✓ Molecular mechanics methods are based on the following principles:
 - Nuclei and electrons are lumped into atom-like particles.
 - Atom-like particles have a net charge
 - Interactions are based on springs and classical potentials.
 - Interactions must be pre-assigned to specific sets of atoms.
- ✓ Interactions determine the spatial distribution of atom-like particles and their energies



Principles Of Molecular Mechanics

AN Whitehead



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