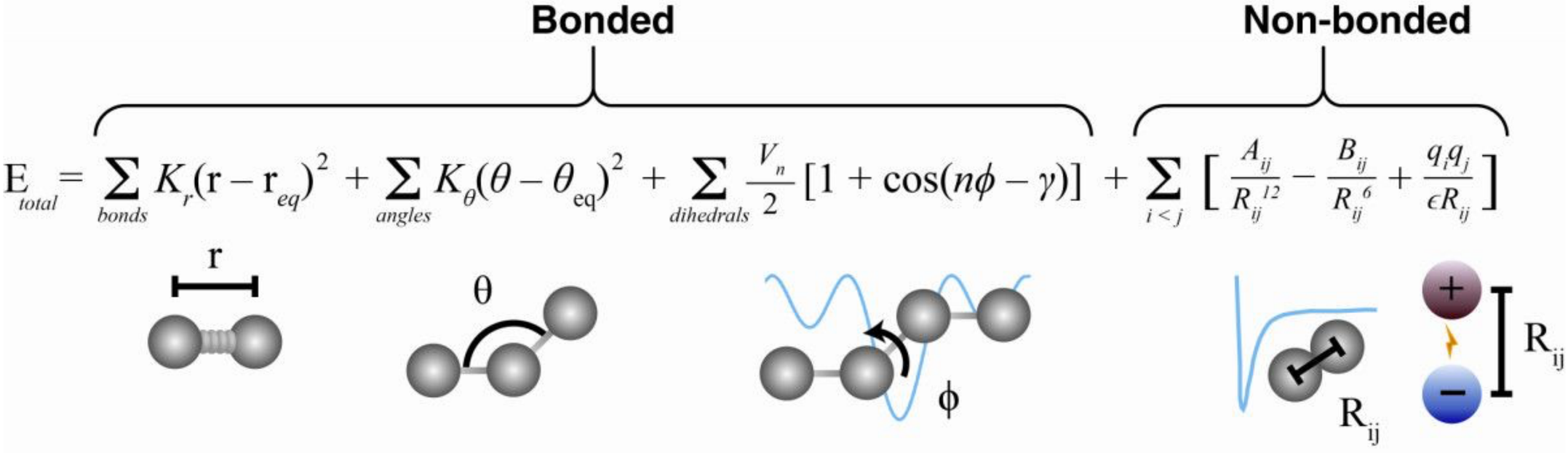
What is Molecular Mechanics?

- Quantum mechanics
  - given the coordinates of atomic nuclei, provides the best description of a system's energy
  - computationally expensive and currently infeasible for biomolecules
- Molecular mechanics
  - treats atoms as hard spheres
  - empirical potential energy
- QM/MM
  - treats part of a system with QM and most with MM
  - in many applications, may balance accuracy and computational speed

- See 1st 45 seconds of "An Introduction to Molecular Dynamics" (https://www.youtube.com/watch?v=lLFEqKl3sm4)

Molecular Mechanics Potential Energy



The potential energy of a system can be divided into those caused by interactions between atoms that are chemically bonded to one another and those caused by interactions between atoms that are not bonded. Chemical bonds and atomic angles are modeled using simple springs, and dihedral angles (that is, rotations about a bond) are modeled using a sinusoidal function that approximates the energy differences between eclipsed and staggered conformations. Non-bonded forces arise due to van der Waals interactions, modeled using the Lennard-Jones potential, and charged (electrostatic) interactions, modeled using Coulomb's law.
Taken from Figure 3 of Durrant & McCammon, 2011.