

# Computational Models

## Molecular Mechanics

- molecule treated as array of atoms governed by a set of classical-mechanical potential functions (e.g., bond stretching is described using a Hooke's Law potential function, i.e., masses attached to springs)
- does not treat electrons explicitly
- absolute energy of a molecule has no intrinsic physical meaning
- parameterized using experimental physical and chemical data for a collection of molecules
- often provides acceptable descriptions of a molecule's equilibrium geometry
- fails for cases where sufficient experimental data do not exist (e.g., short-lived reactive intermediates, transition states, reaction pathways)
- used for preliminary refinement of geometry, and conformational searching
- relative computational speed = fast

## Semi-Empirical

- involves an approximate solution to the quantum-mechanical Schrodinger equation (the Schrodinger equation cannot be solved exactly for many-electron systems)
- treats only valence-shell atomic orbitals and electrons
- parameterized using experimental physical and chemical data for a collection of molecules
- can produce meaningful, often quantitative, results for large molecular systems
- generally more applicable and more reliable than Molecular Mechanics
- relative computational speed = fast to moderate

## Ab Initio

- involves an approximate solution to the quantum-mechanical Schrodinger equation
- treats *all* atomic orbitals and electrons
- includes parametrization *only for elements* using experimental data
- can produce remarkably accurate, quantitative results - but molecular size can be a limitation
- generally more applicable and more reliable than either Molecular Mechanics or Semi-Empirical models
- relative computational speed = moderate to slow

***The results obtained using these computational models are for molecules in the gas phase at absolute zero (0 K). For very accurate work, corrections must be applied.***