

# Background & motivation for MD simulations

- Biological structures and events (functions) do not occur at absolute zero...
- Thermal “*wiggling and jiggling of atoms*” is vital to both biological **structure** and **function**
- Evolution selects for function, which arises from sequence and structure... and dynamics!
- Folding pathway of a small protein
- Assembly pathway of a “molecular machine” (ribosomal subunits)

