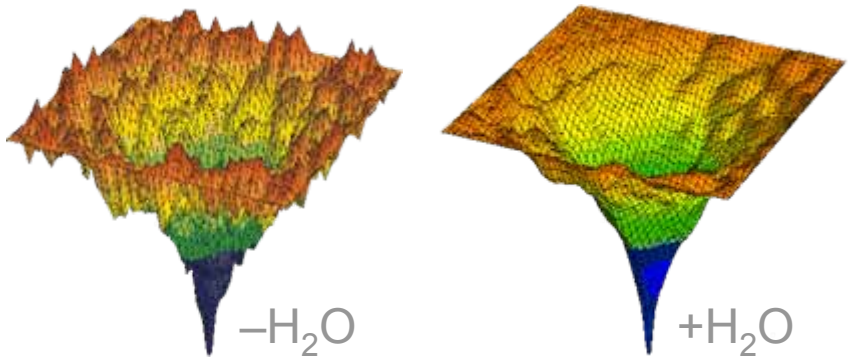
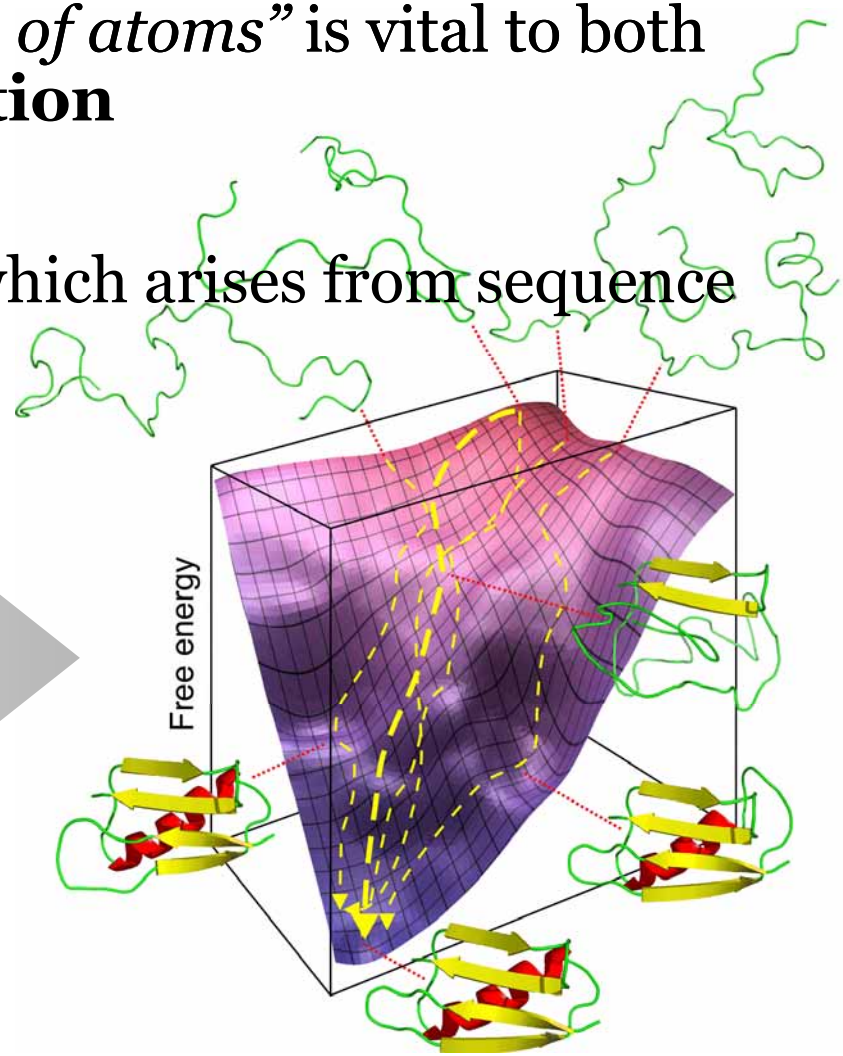
Background & motivation for MD simulations

- 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**
  and **function**
- Evolution selects for function, which arises from sequence
  and structure… and dynamics!
  and structure…
  and dynamics!
- Folding pathway**s**
  of a small protein





Cameron Mura; May 2007