

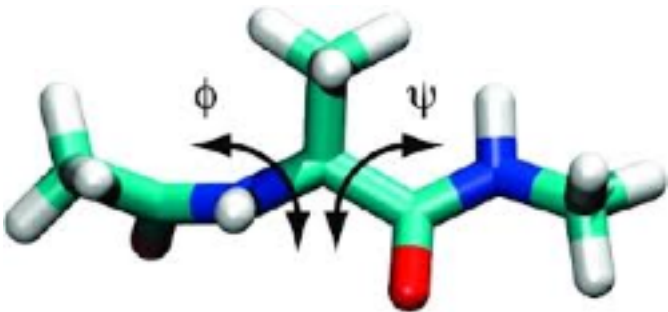
EXAMPLE: MOLECULAR DYNAMICS

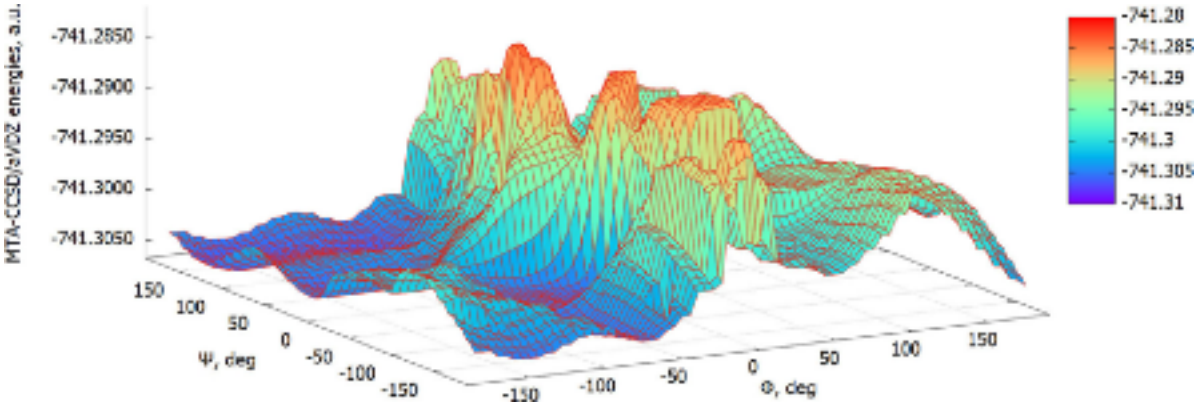
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► Molecular dynamics simulates these systems to infer physical properties



Potential energy molecular potentials, molecular potentials, potentials



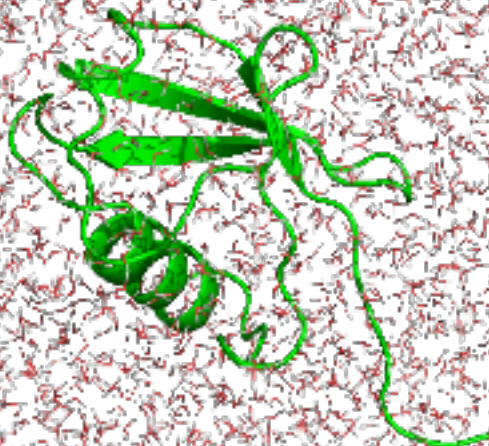


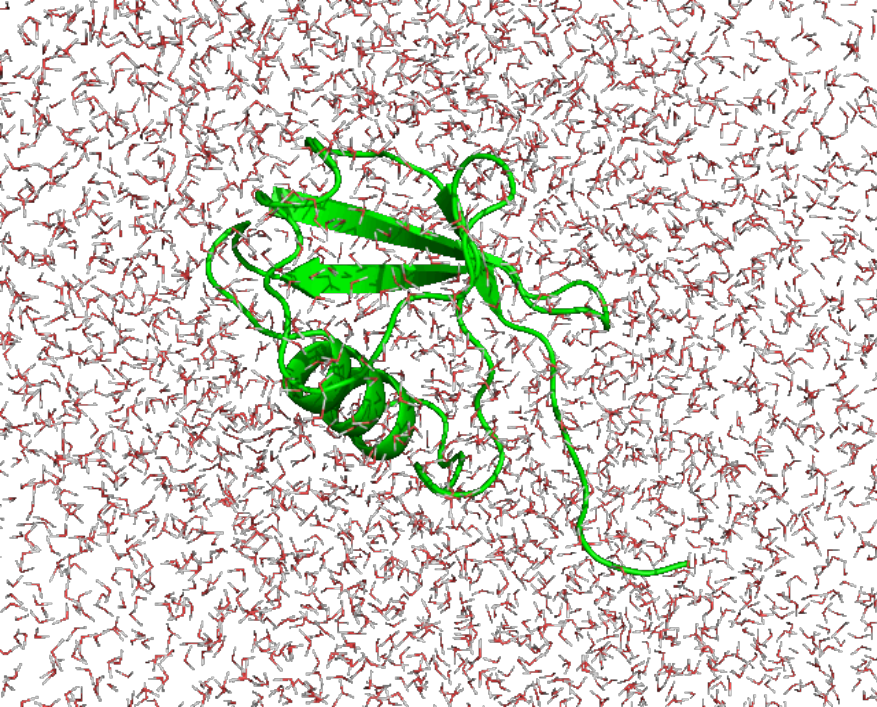
State represents different configurations of a system of particles



► Estimate reactions rates, binding affinity, material properties, etc

very important for driving discovery

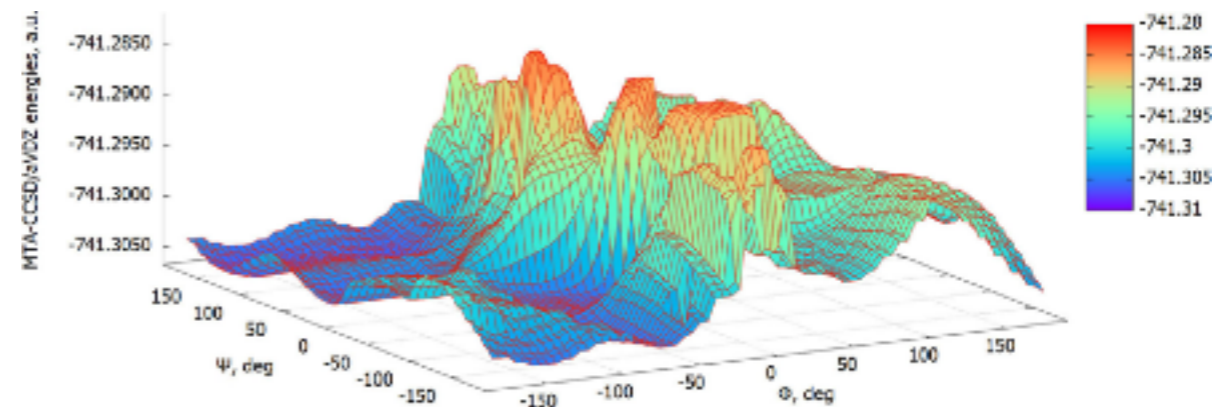
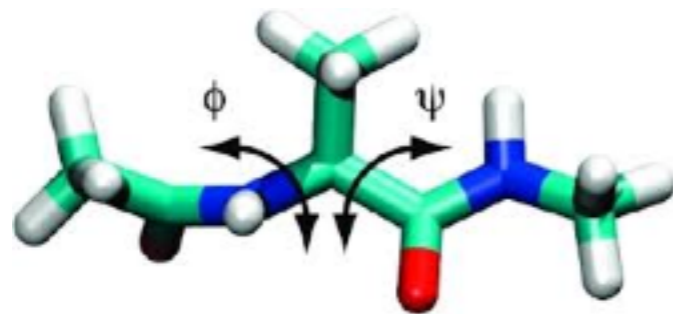




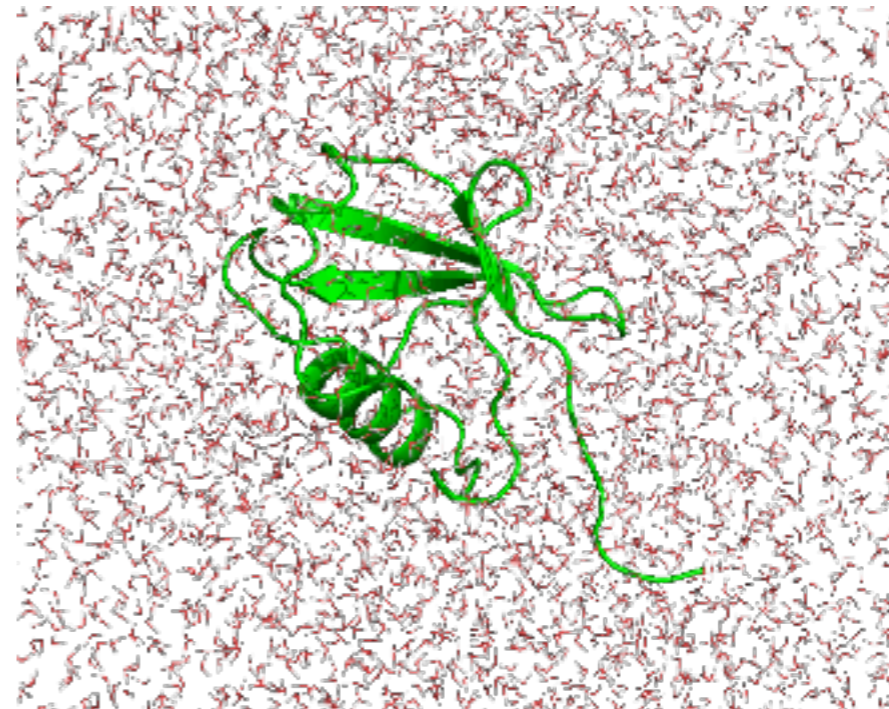
EXAMPLE: MOLECULAR DYNAMICS

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- ▶ Statespace represents different configurations of a system of particles
- ▶ Potential encodes the molecular forces between atoms, molecules, proteins etc



- ▶ Molecular dynamics simulates these systems to infer physical properties
- ▶ Estimate reactions rates, binding affinity, material properties, etc
- ▶ Very important for drug discovery



EXAMPLE: QUANTUM CHROMODYNAMICS