

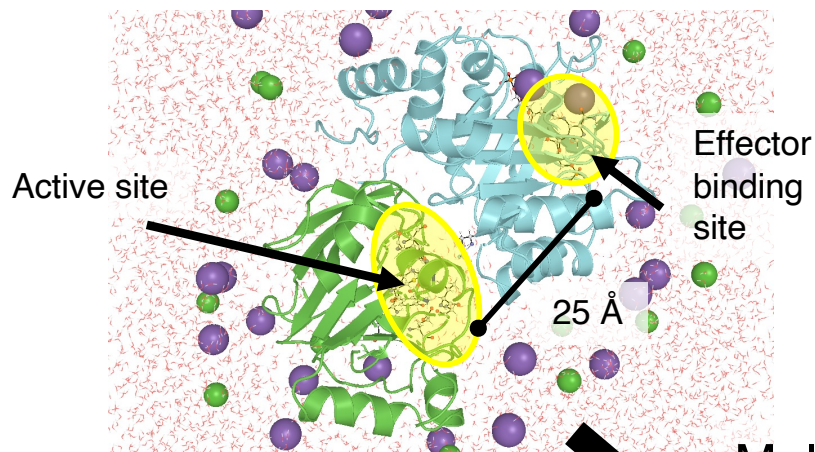
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How is enzyme catalysis influenced by allosteric regulation (regulation from a distance)?

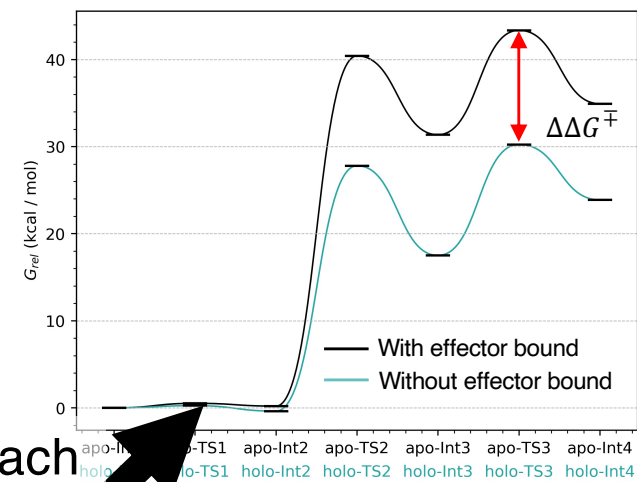
Classical mechanics

used to describe molecular motion



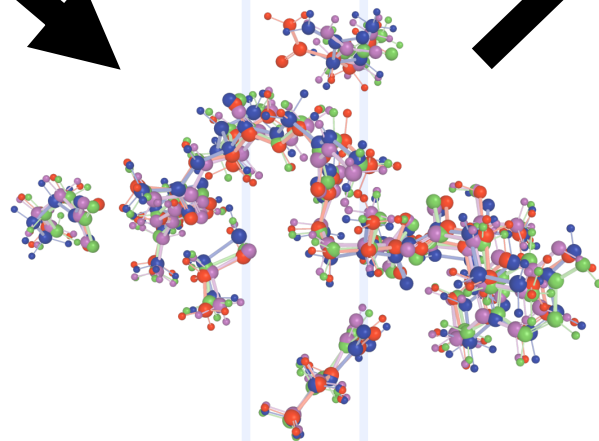
Quantum mechanics

used to describe electronic motion



Multiscale Approach

- Molecular dynamics provides time evolution of atoms (trajectory)
- **Current work:** developing a structural clustering algorithm to classify relevant conformations



- Density functional theory provides reaction profile based on optimized geometries of reaction species
- **Current work:** modeling enzyme active site to calculate energy barrier

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- No formal background in CS
 - Wrote my first program only 2 years ago
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- Gain a better understanding of HPC resources in order to best utilize them
 - Implement optimization strategies and sustainable code (version control) practices

Paton Research Group (CSU)



McCullagh Research Group (OSU)



Thanks for organizing the Summer Institute @ SDSC!