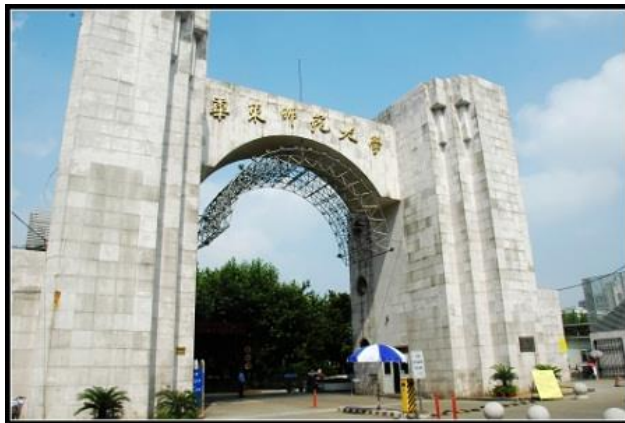


2014 NYU&ECNU Symposium for Undergraduate Research

Simulation of Biochemical Reactions in Proteins

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Introduction



2007, Xiamen



2007, Shanghai



2009, Heidelberg



2011, Singapore

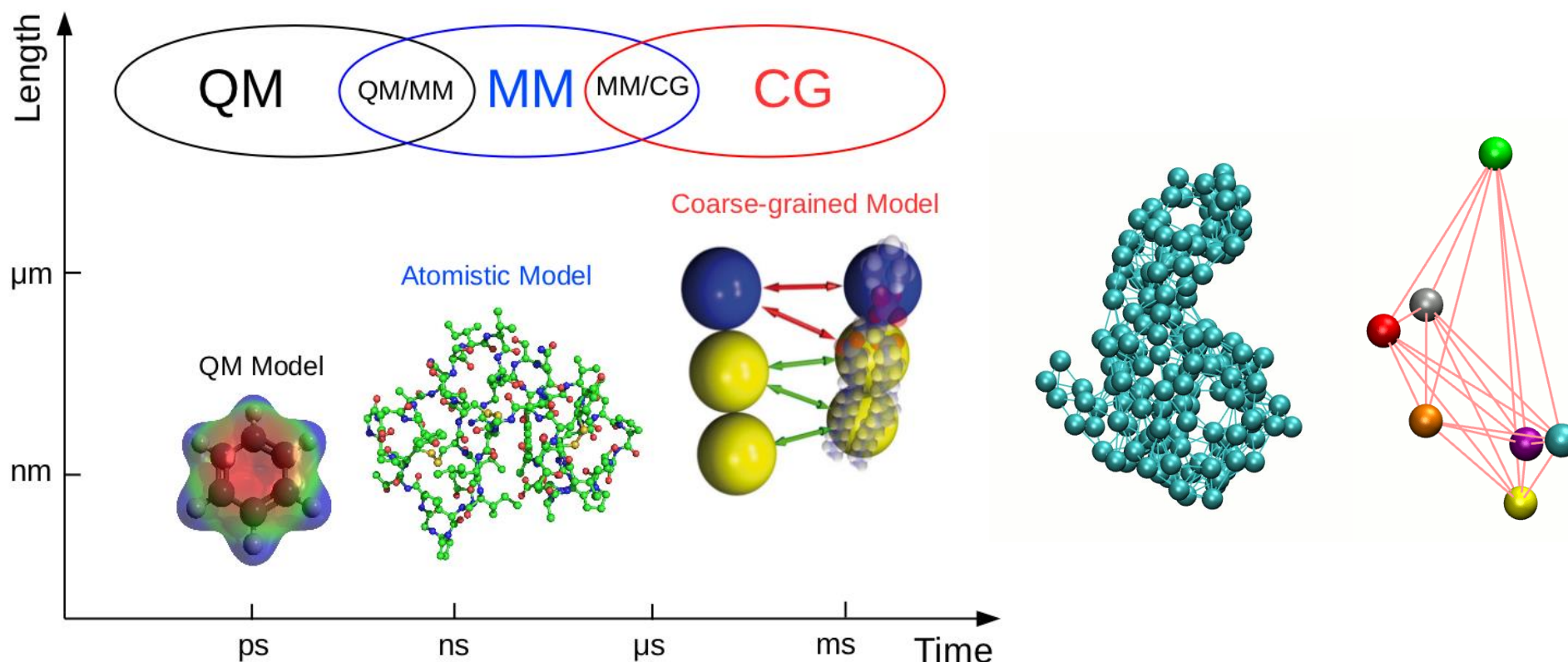


2014, ECNU



When and where ?

Multiscale Simulations of Biochemical Systems



Outline

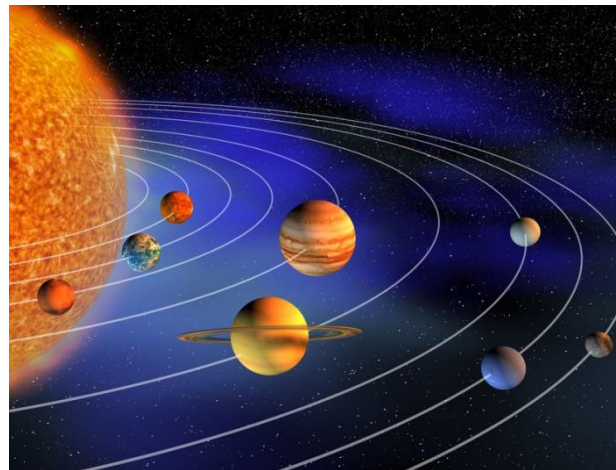
- Background of Quantum Mechanics
- Description of Simple Chemical Reactions
- Simulation of Chemical Reactions in Proteins

Motions of Microparticles

Classical Mechanics:

Newton's second law:

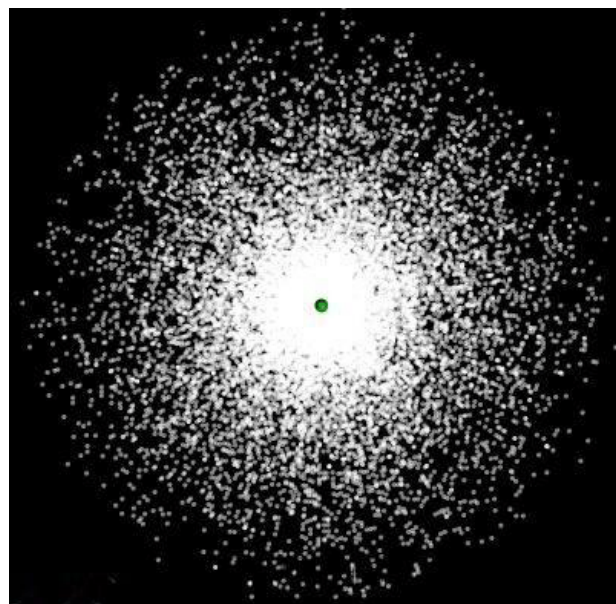
$$F = ma$$



Quantum Mechanics:

Schrödinger equation:

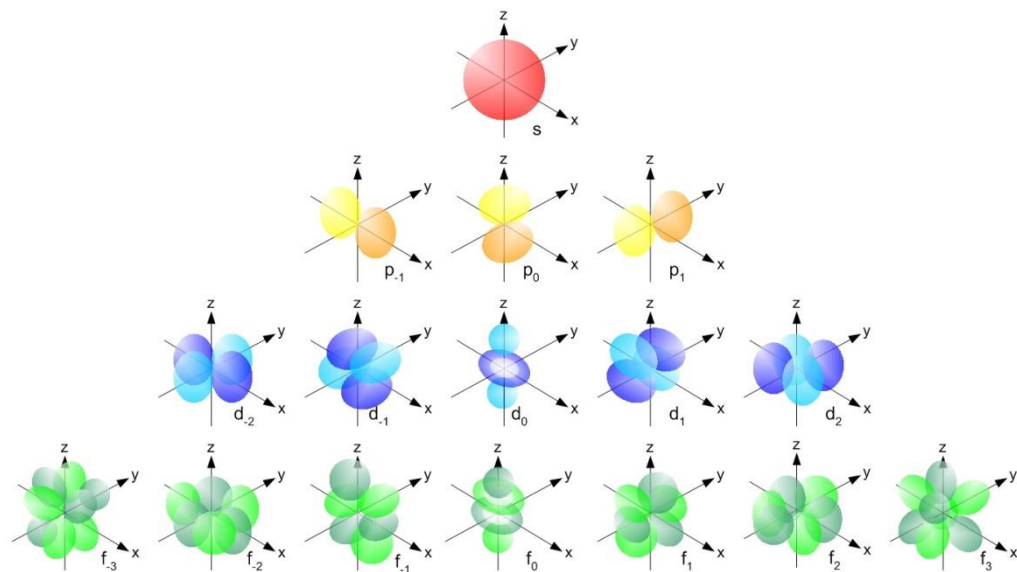
$$\left(-\frac{\hbar^2}{2m} \nabla^2 + \hat{V} \right) \psi = E\psi$$



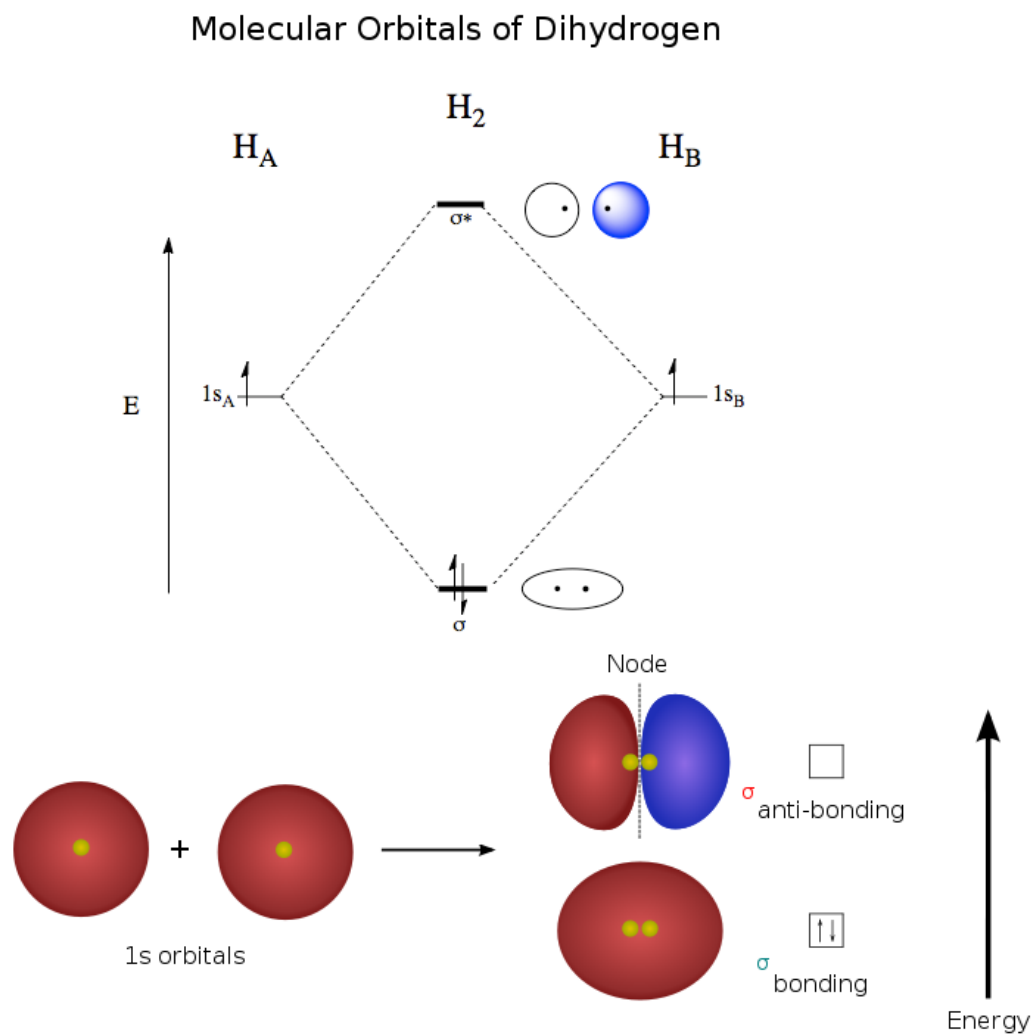
Atomic Orbitals(AO) of Hydrogen Atom



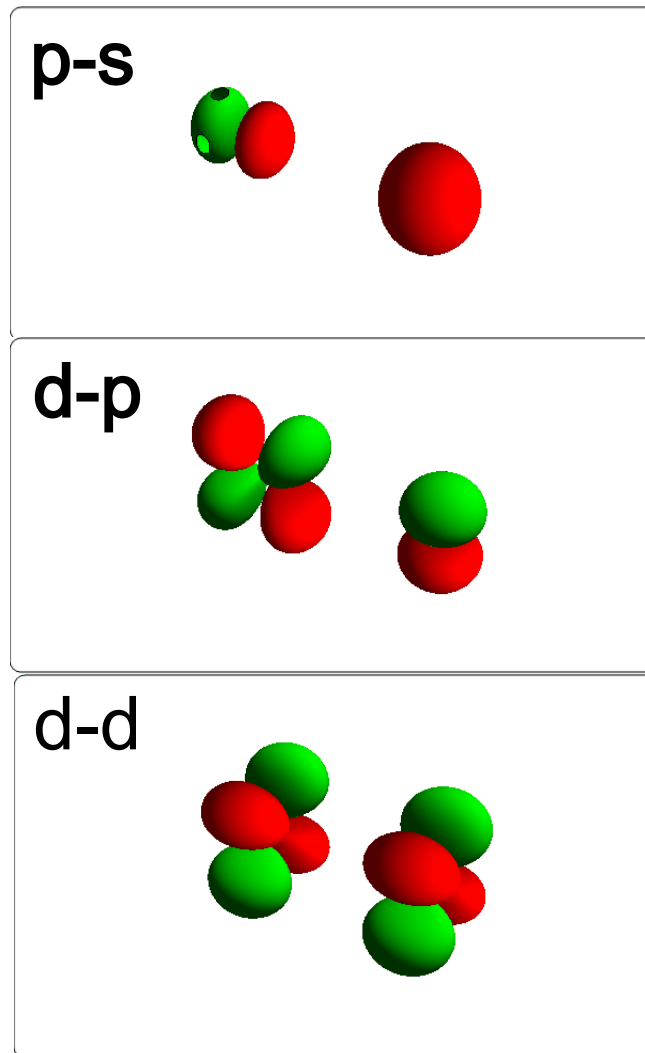
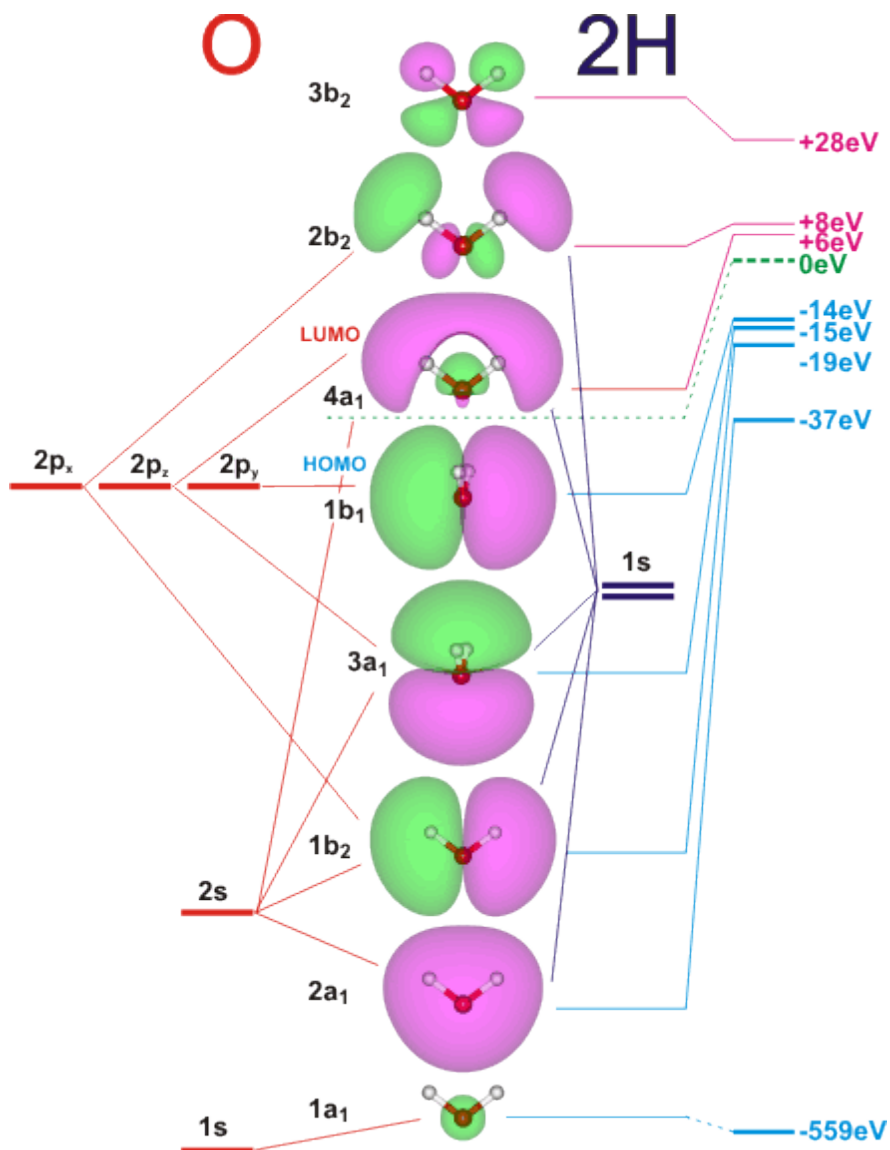
$n=1 \quad l=0 \quad m=0 \quad \Psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-\rho}$	HYDROGEN-ATOM WAVE FUNCTIONS, $n \leq 3$ $\rho \equiv \frac{r}{a_0}$
$n=2 \quad l=0 \quad m=0 \quad \Psi_{200} = \frac{1}{8} \left(\frac{2}{\pi a_0^3}\right)^{1/2} (2-\rho)e^{-\rho/2}$	
$n=2 \quad l=1 \quad m=0 \quad \Psi_{210} = \frac{1}{8} \left(\frac{2}{\pi a_0^3}\right)^{1/2} \rho e^{-\rho/2} \cos \theta$	
$n=2 \quad l=1 \quad m=\pm 1 \quad \Psi_{211} = \frac{1}{8} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho e^{-\rho/2} \sin \theta e^{i\phi}$	$\Psi_{21-1} = \frac{1}{8} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho e^{-\rho/2} \sin \theta e^{-i\phi}$
$n=3 \quad l=0 \quad m=0 \quad \Psi_{300} = \frac{1}{243} \left(\frac{3}{\pi a_0^3}\right)^{1/2} (27-18\rho+2\rho^2)e^{-\rho/3}$	
$n=3 \quad l=1 \quad m=0 \quad \Psi_{310} = \frac{1}{81} \left(\frac{2}{\pi a_0^3}\right)^{1/2} \rho(6-\rho)e^{-\rho/3} \cos \theta$	
$n=3 \quad l=1 \quad m=\pm 1 \quad \Psi_{311} = \frac{1}{81} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho(6-\rho)e^{-\rho/3} \sin \theta e^{i\phi}$	$\Psi_{31-1} = \frac{1}{81} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho(6-\rho)e^{-\rho/3} \sin \theta e^{-i\phi}$
$n=3 \quad l=2 \quad m=0 \quad \Psi_{320} = \frac{1}{486} \left(\frac{6}{\pi a_0^3}\right)^{1/2} \rho^2 e^{-\rho/3} (3\cos^2 \theta - 1)$	
$n=3 \quad l=2 \quad m=\pm 1 \quad \Psi_{321} = \frac{1}{81} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho^2 e^{-\rho/3} \sin \theta \cos \theta e^{i\phi}$	$\Psi_{32-1} = \frac{1}{81} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho^2 e^{-\rho/3} \sin \theta \cos \theta e^{-i\phi}$
$n=3 \quad l=2 \quad m=\pm 2 \quad \Psi_{322} = \frac{1}{162} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho^2 e^{-\rho/3} \sin^2 \theta e^{i2\phi}$	$\Psi_{32-2} = \frac{1}{162} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \rho^2 e^{-\rho/3} \sin^2 \theta e^{-i2\phi}$



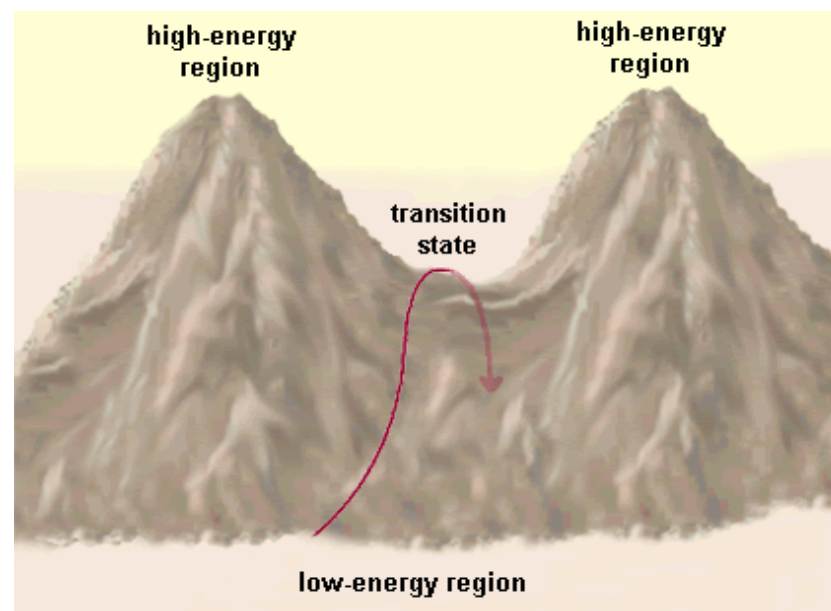
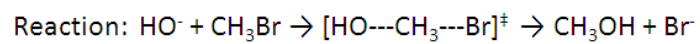
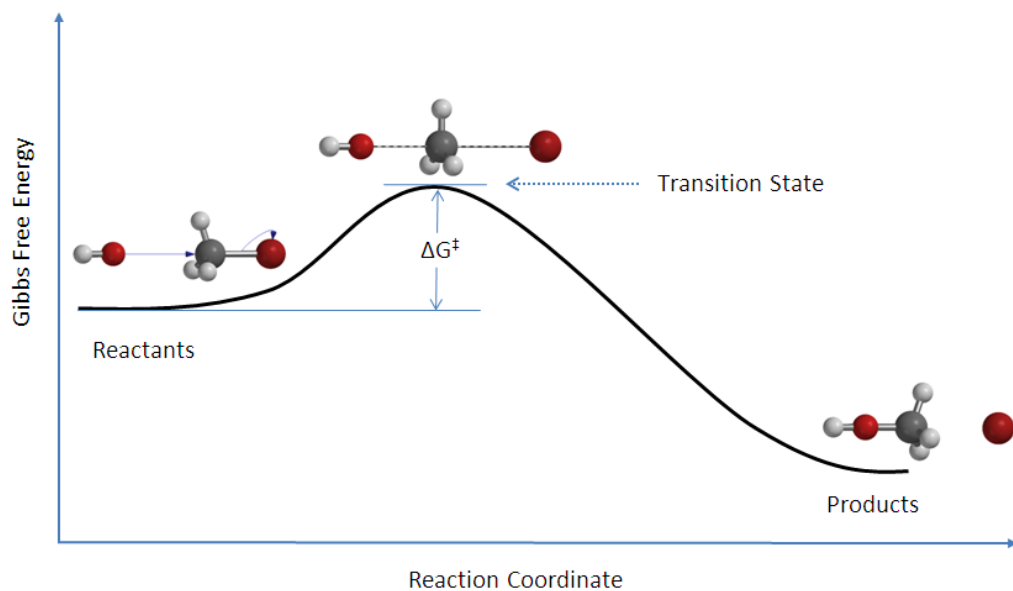
Molecular Orbitals(MO) of Dihydrogen Molecule



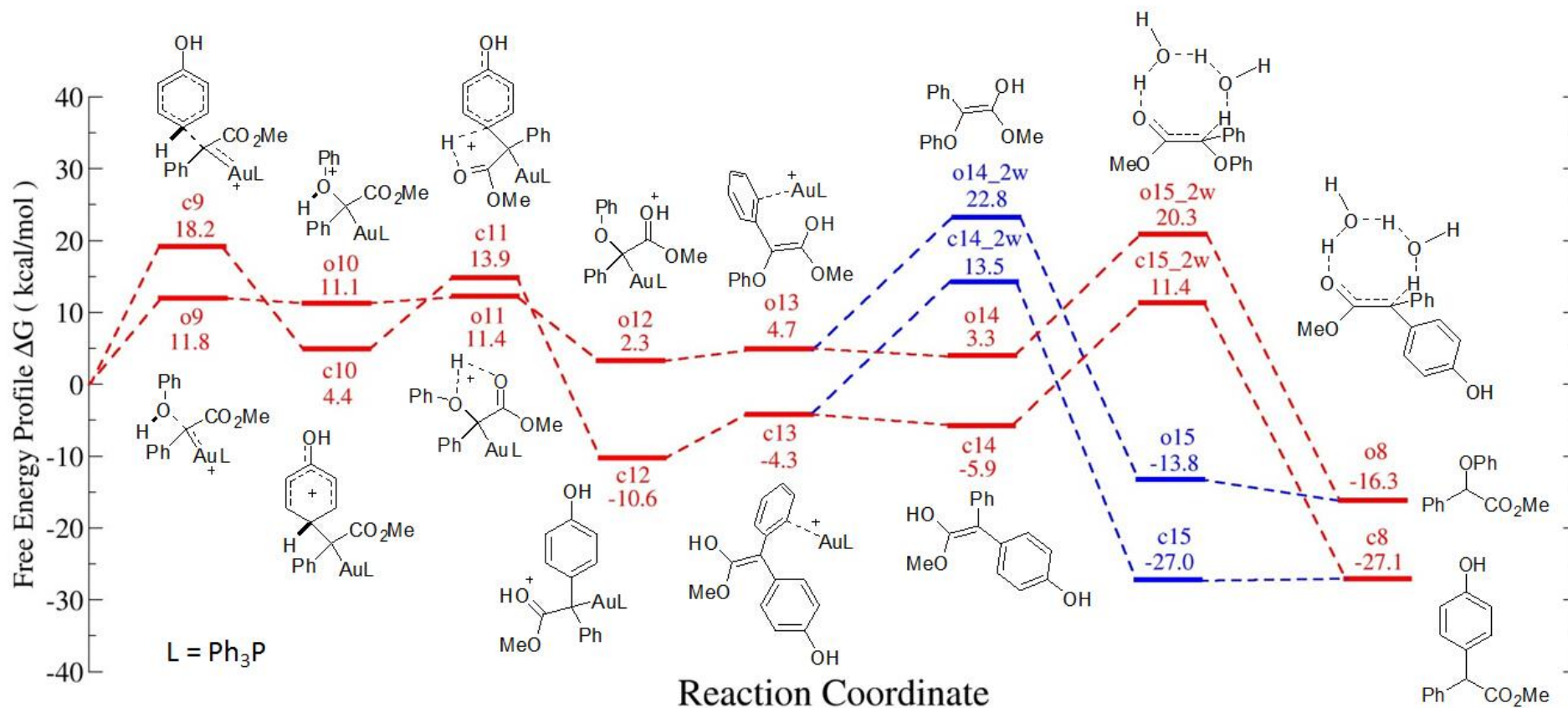
Molecular Orbitals(MO) of H₂O



Transition State Theory

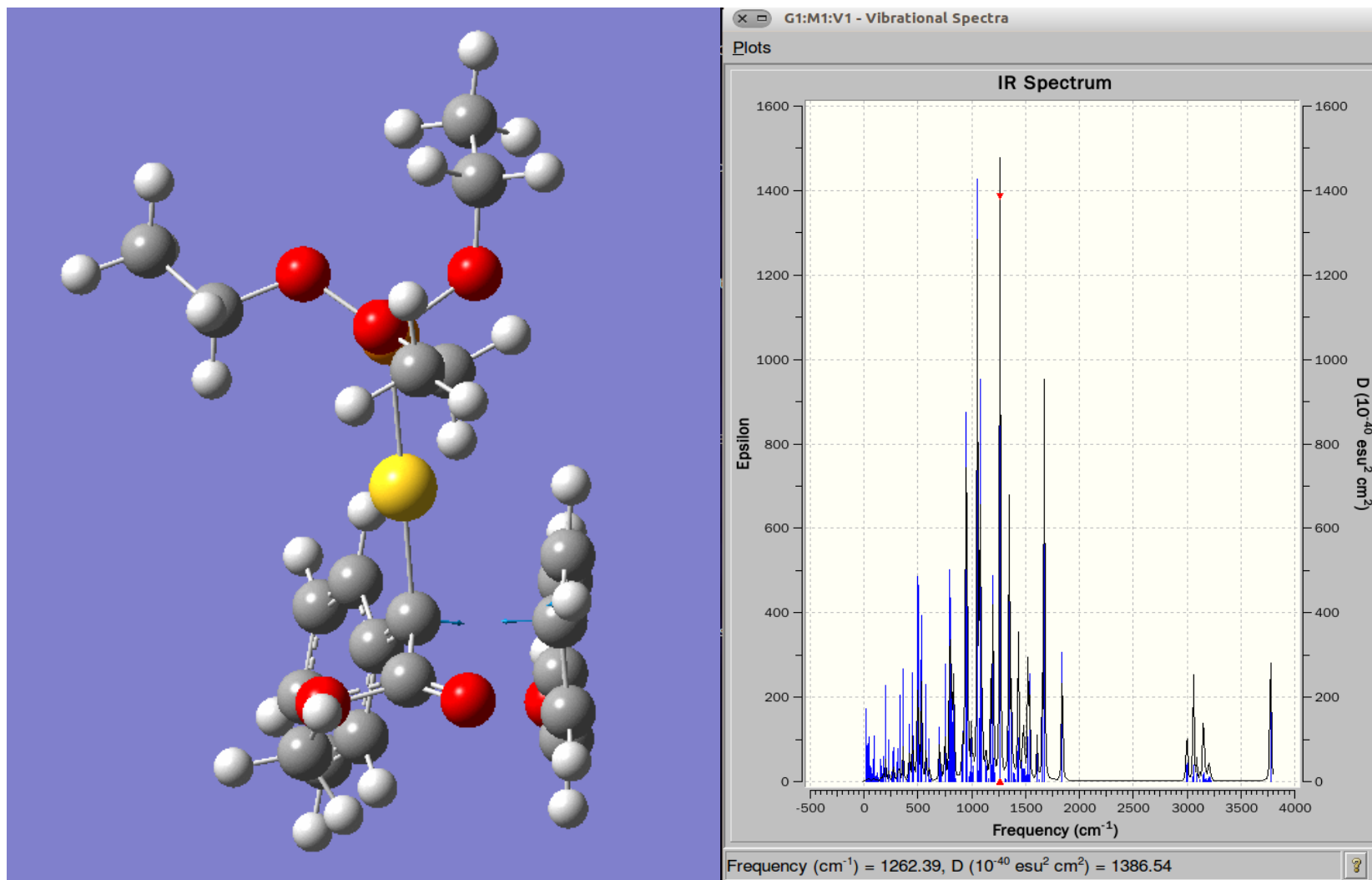


Theoretical Pathways of Organometallic Reactions



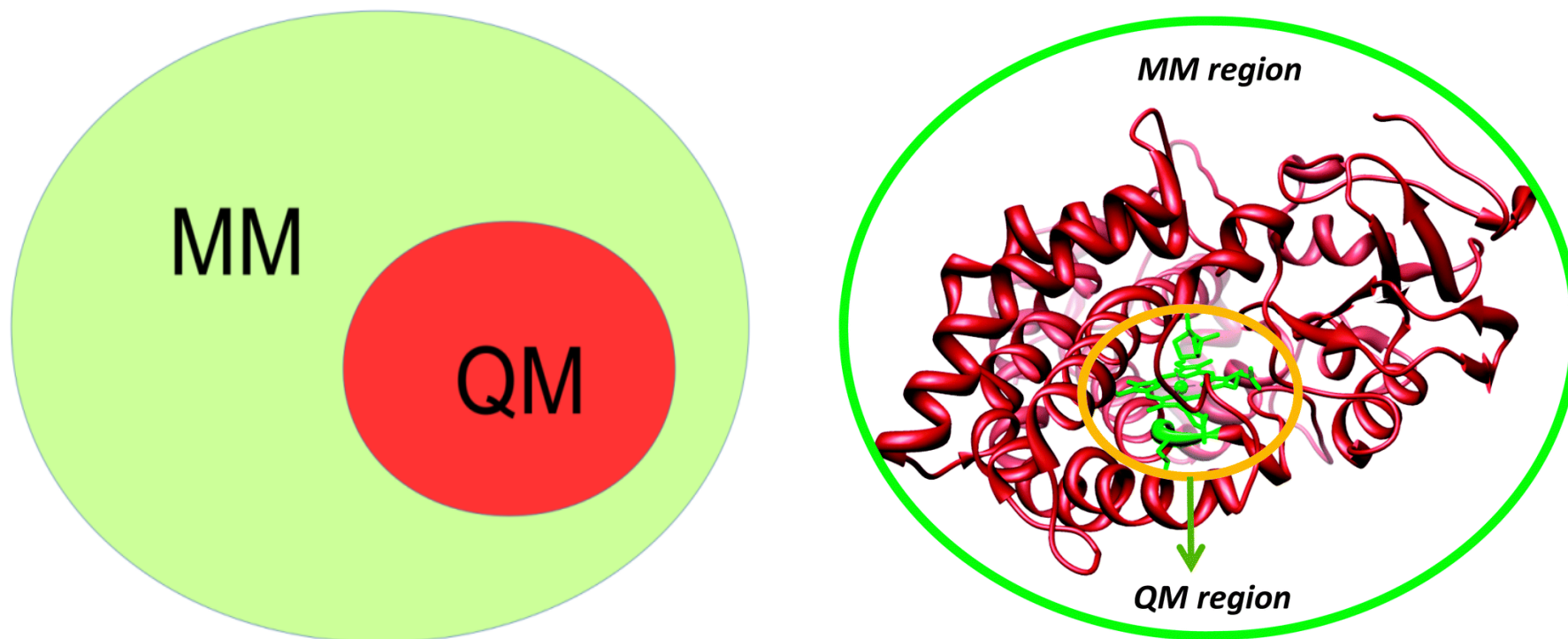
Fei Xia's study

Transition State and IR Vibrations



Fei Xia's study

QM/MM Simulation of Chemical Reactions in Proteins

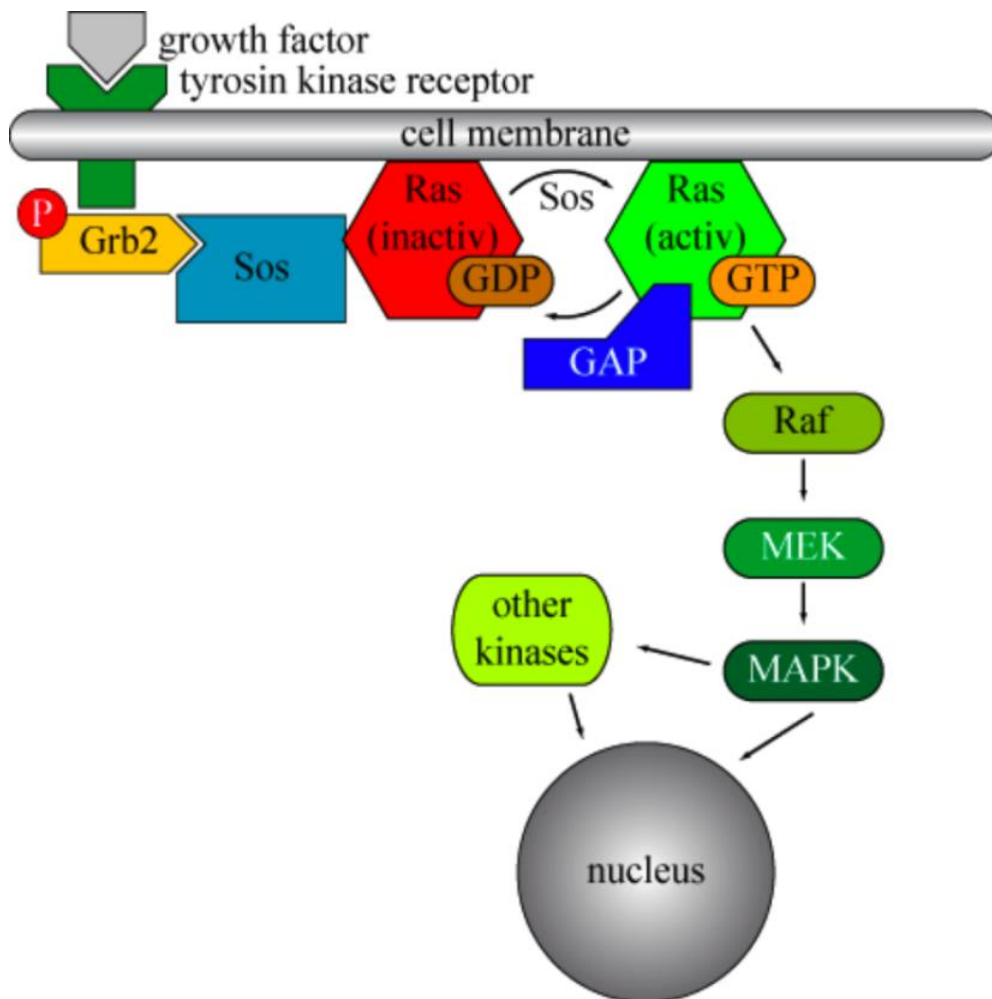


QM: quantum mechanics methods

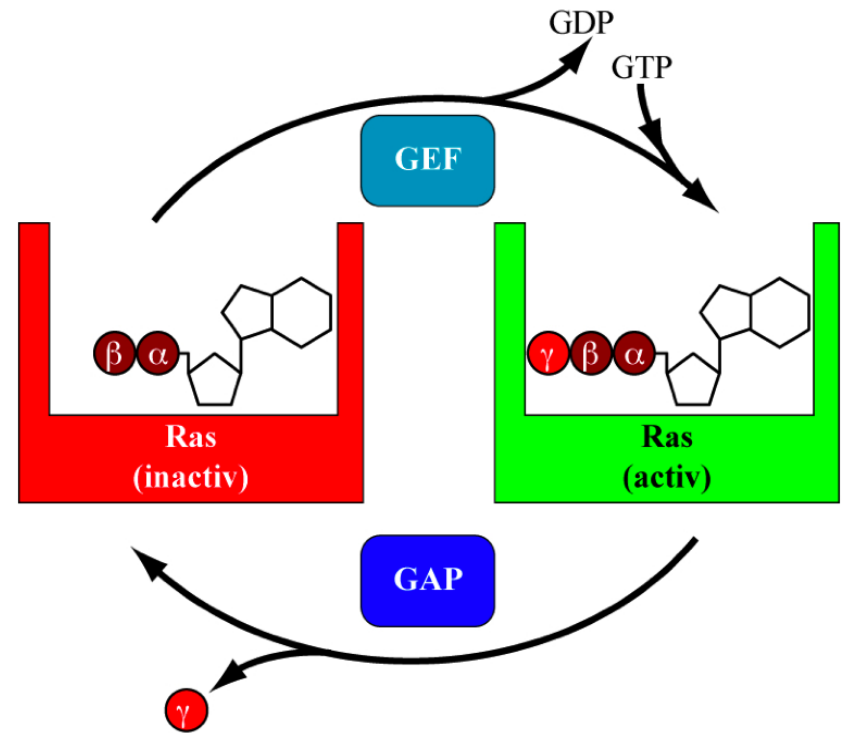
MM: molecular mechanics methods

Function of Ras Protein

Ras/Raf/MAPK Pathway

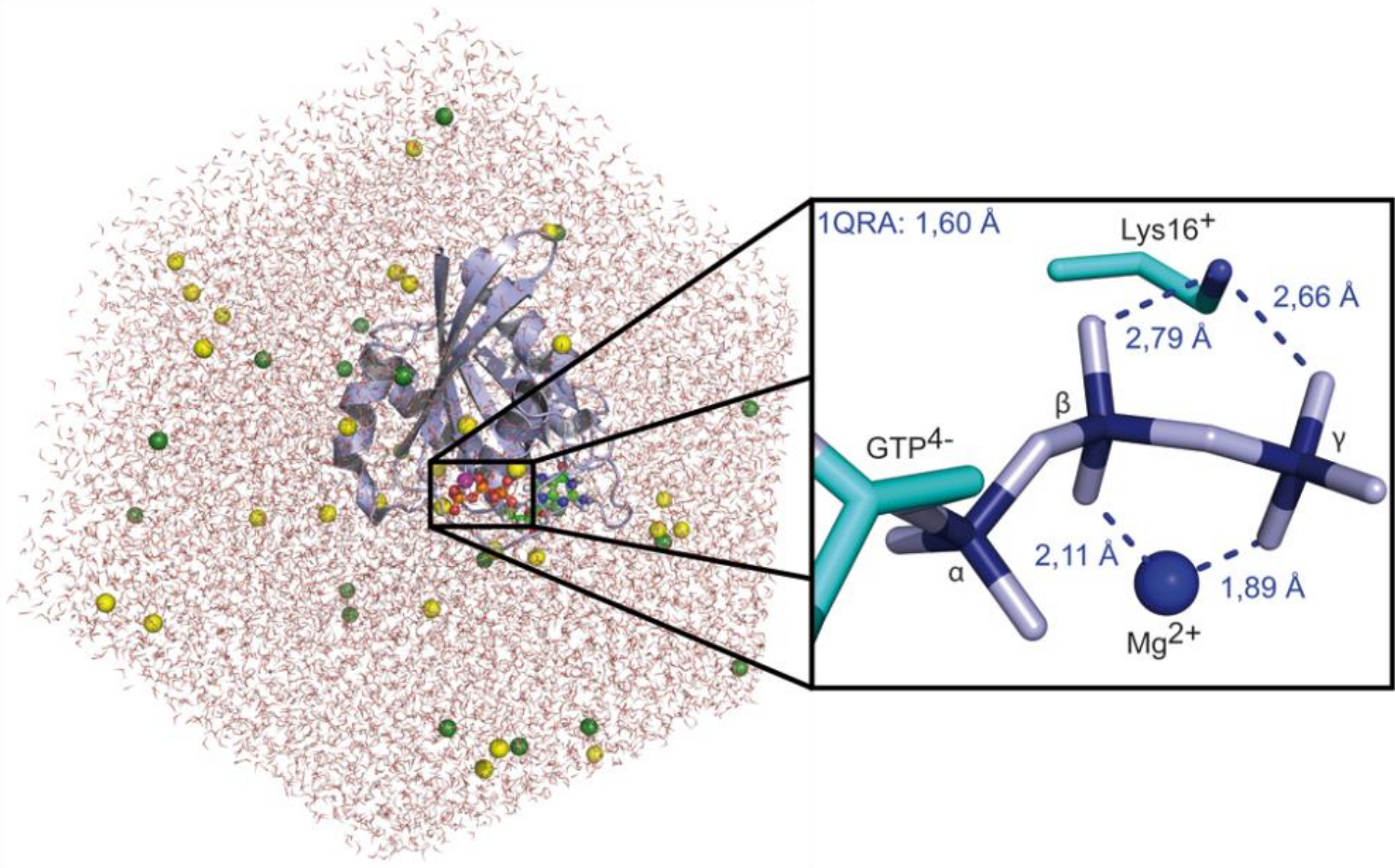


GTP/GDP Cycle

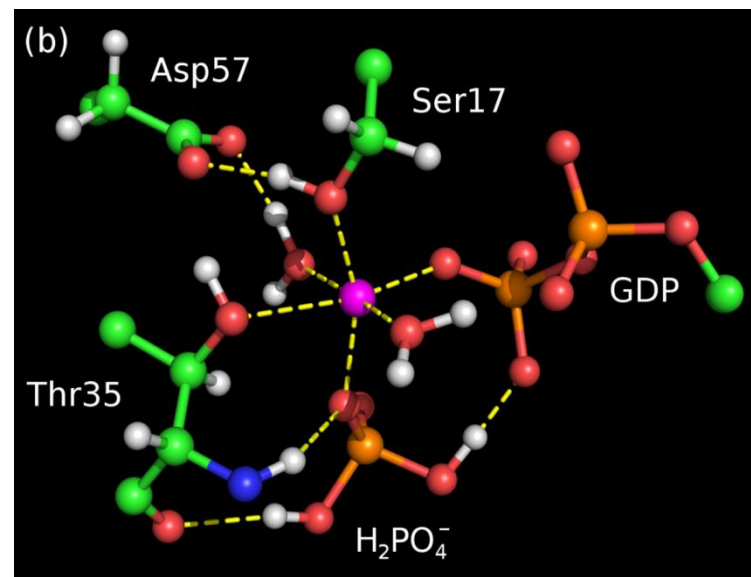
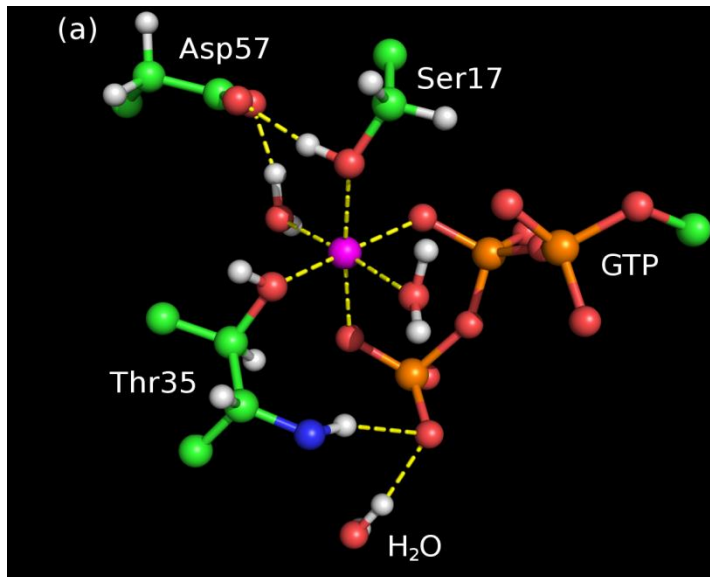
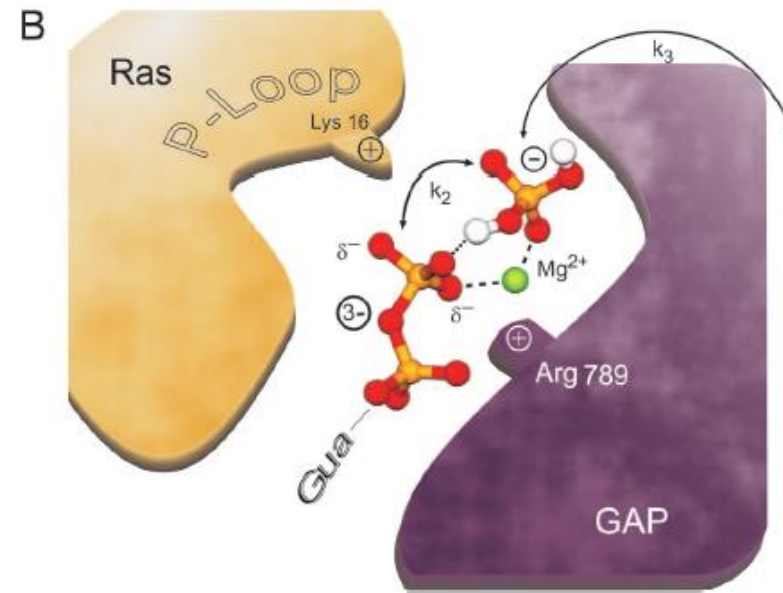
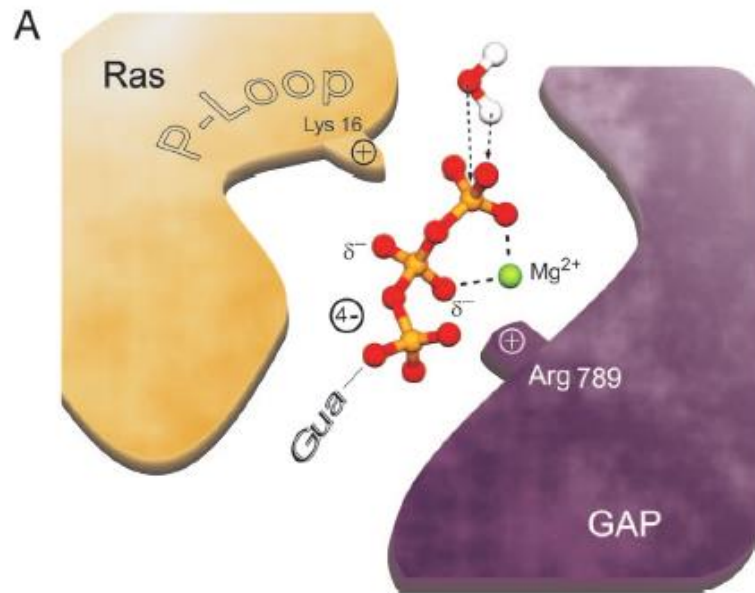


GTP: guanosine triphosphate
GDP: guanosine diphosphate
GEF: guanine exchange factor
GAP: GTPase-activating protein

The QM/MM Simulation



Reaction Mechanism of GTP to GDP



Thank you for your attentions!