# Simulation of Biochemical Reactions in Proteins

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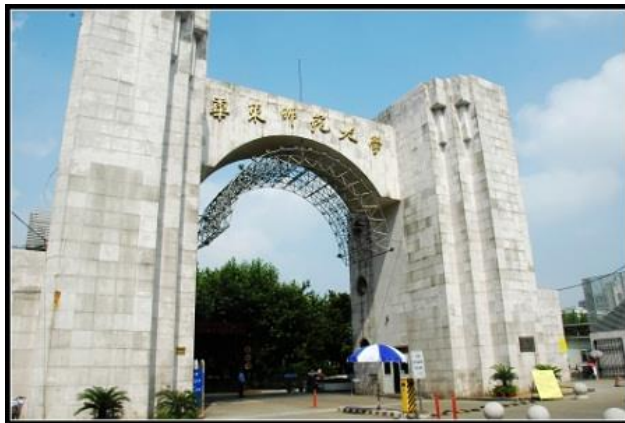
# Introduction



2007, Xiamen
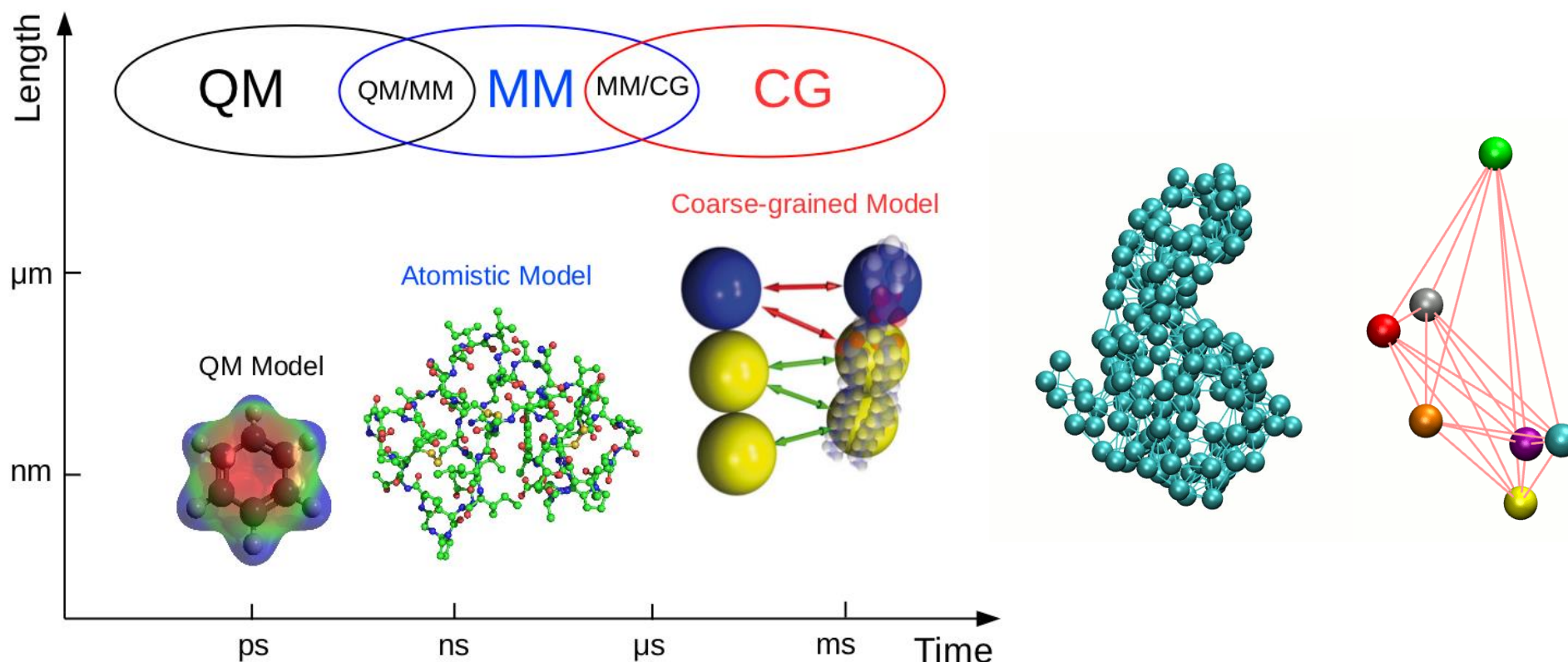
2007, Shanghai

2009, Heidelberg

2011, Singapore

2014, ECNU

When and where ?

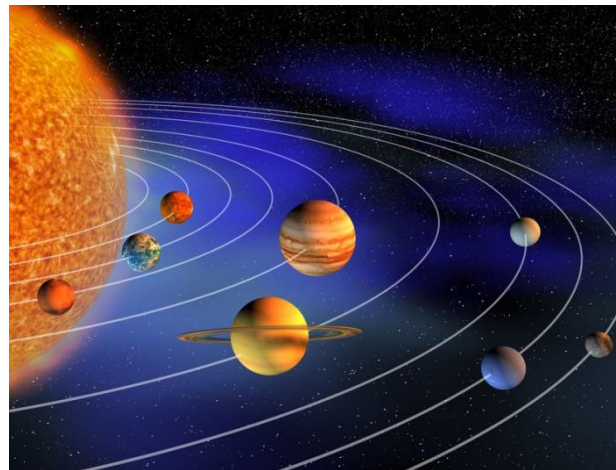# Multiscale Simulations of Biochemical Systems

# Outline

- ➢ Background of Quantum Mechanics

- ➢ Description of Simple Chemical Reactions

- ➢ Simulation of Chemical Reactions in Proteins

# Motions of Micropaticles
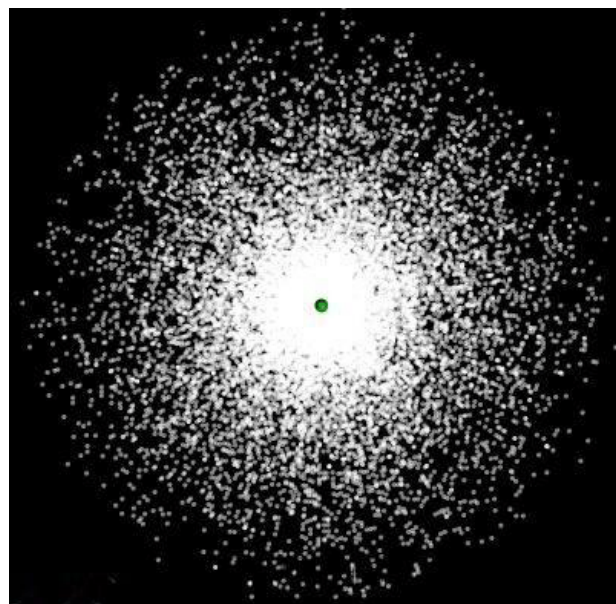
## Classical Mechanics:

Newton's second law:

$$F = ma$$
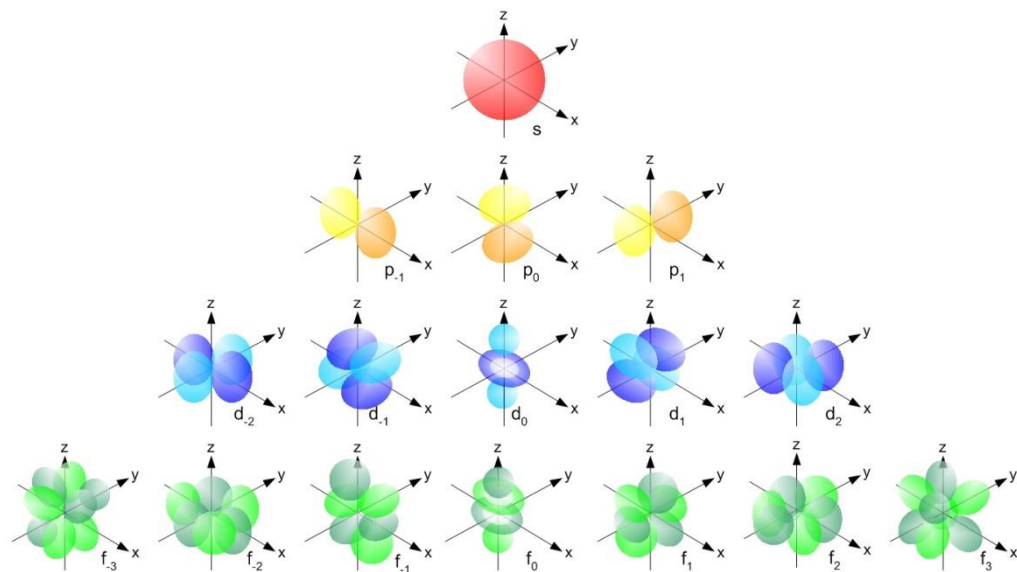


## Quantum Mechanics:

Schrödinger equation:

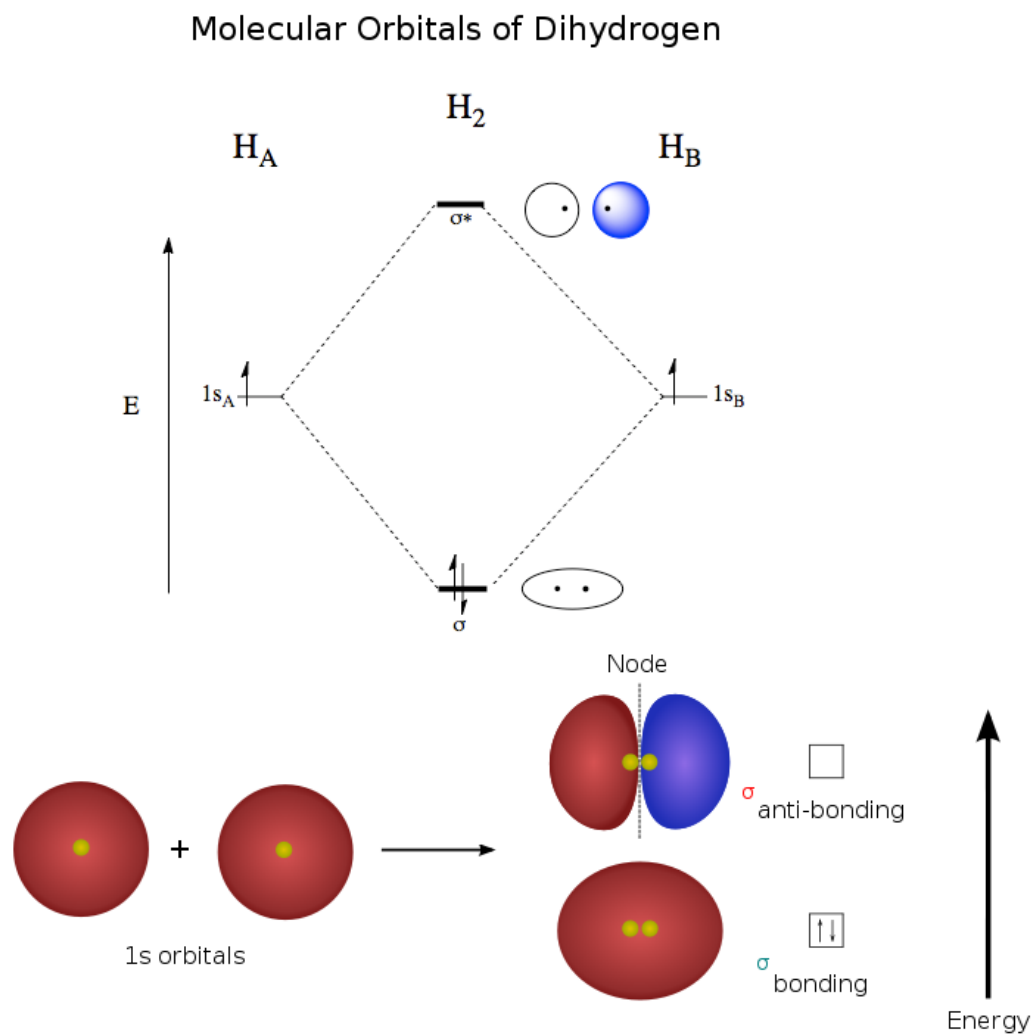$$\left( -\frac{h^2}{8\pi^2 m} \nabla^2 + \hat{V} \right) \psi = E\psi$$
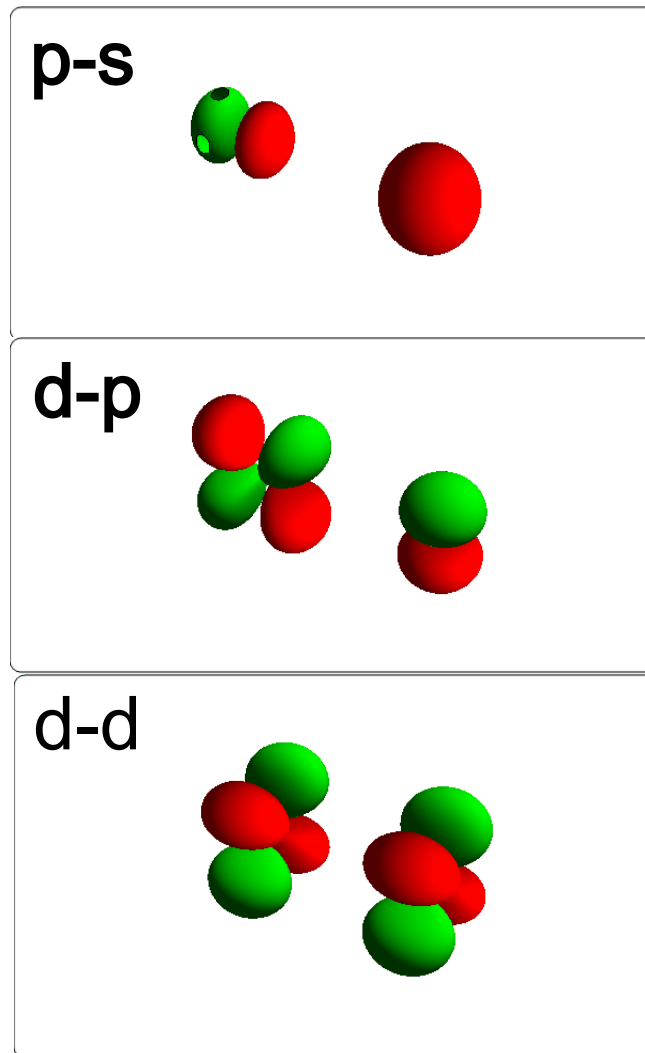
# Atomic Orbitals(AO) of Hydrogen Atom

# Molecular Orbitals(MO) of Dihydrogen Molecule
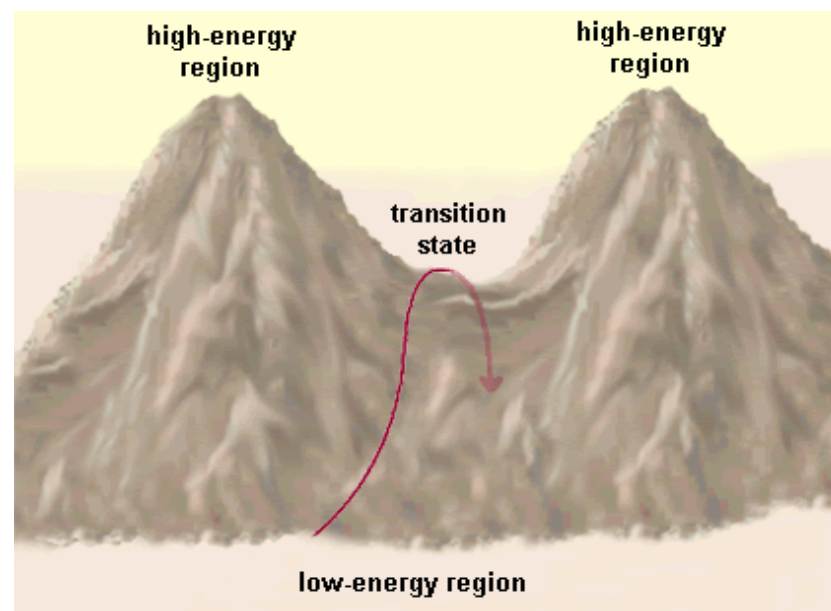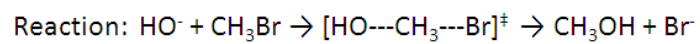


Molecular Orbitals of Dihydrogen

# Molecular Orbitals(MO) of H$_2$O
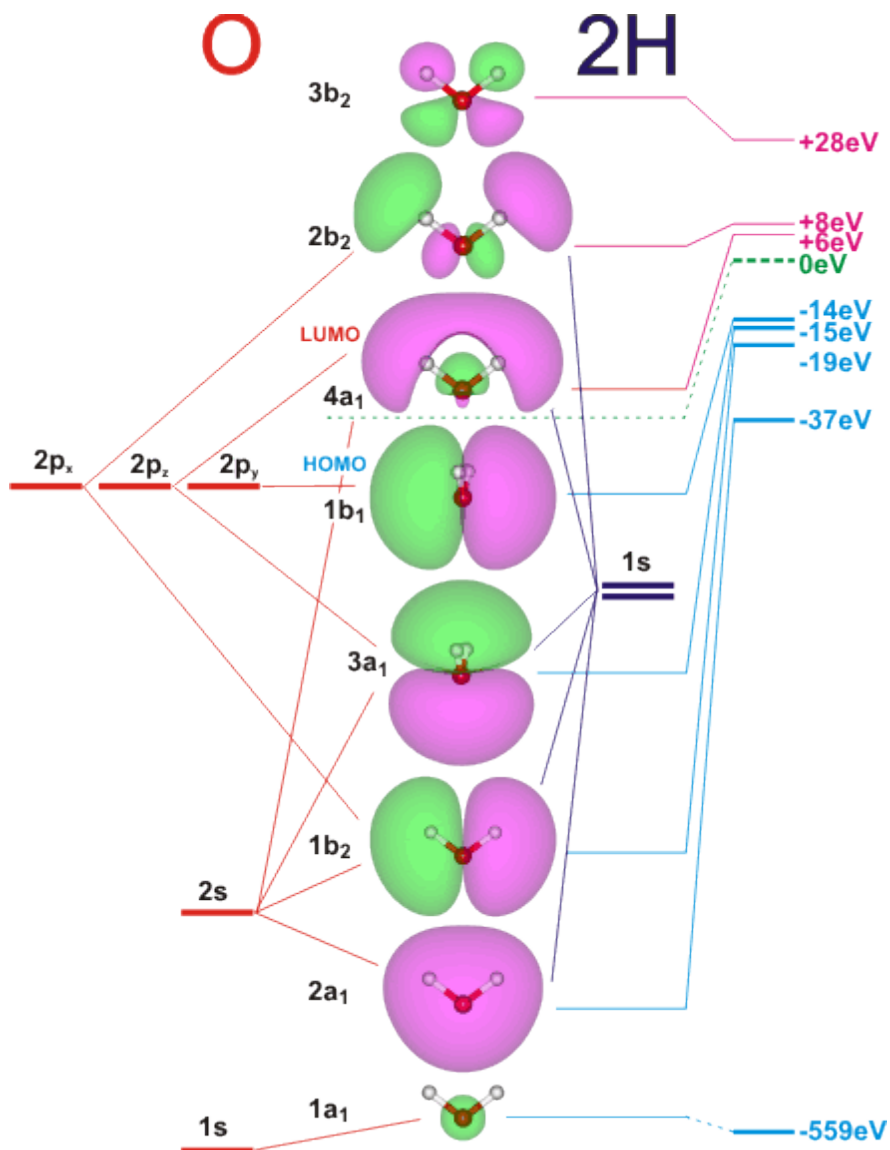
# Transition State Theory



Reaction: $HO^- + CH_3Br \rightarrow [HO\text{---}CH_3\text{---}Br]^\ddagger \rightarrow CH_3OH + Br^-$
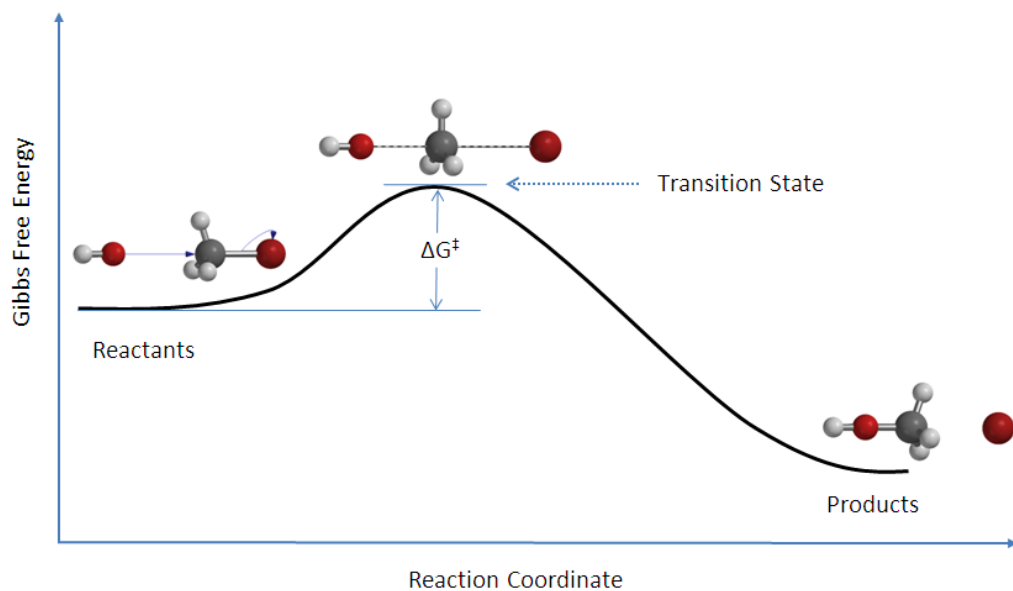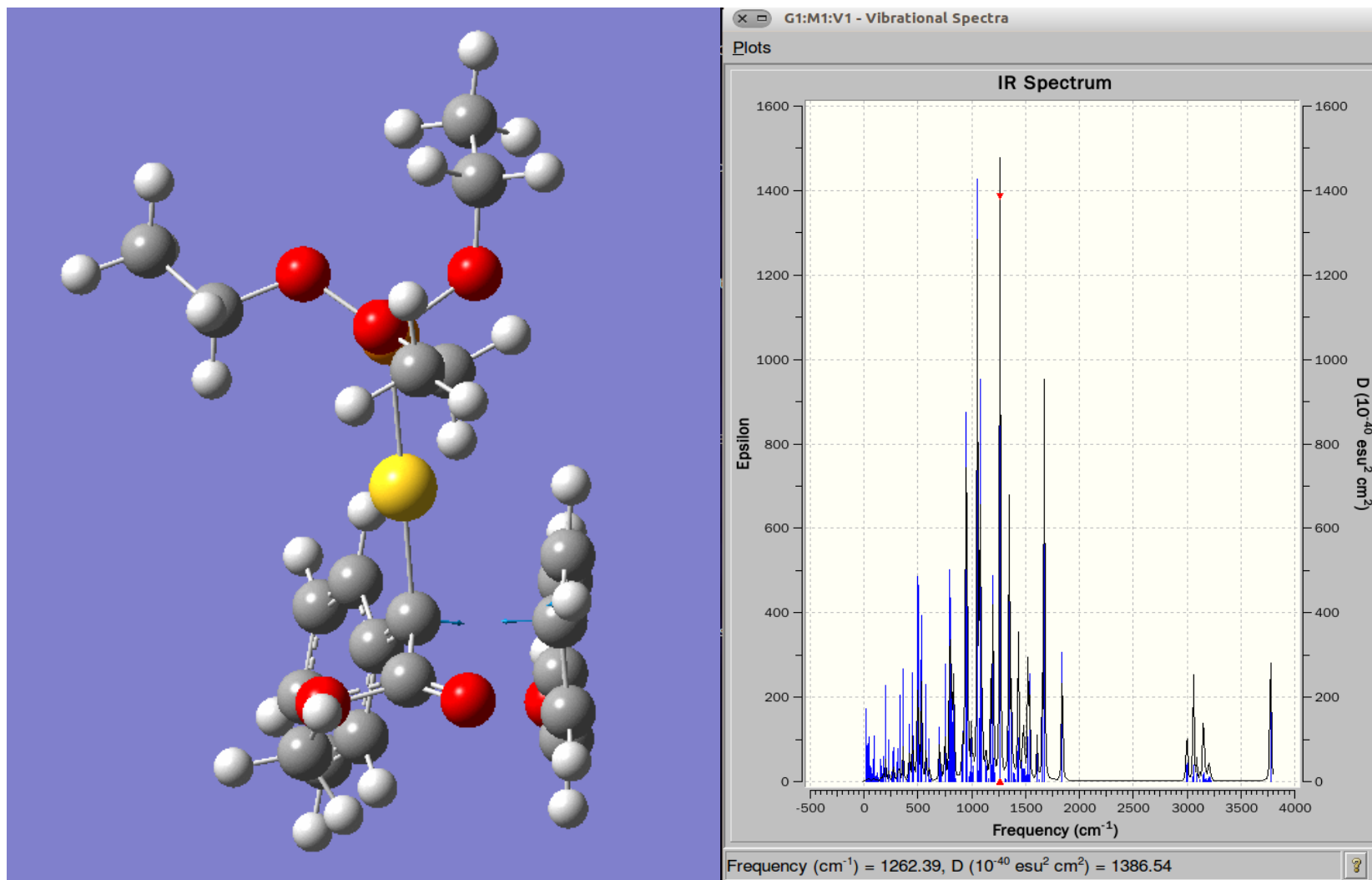
# Theoretical Pathways of Organometallic Reactions
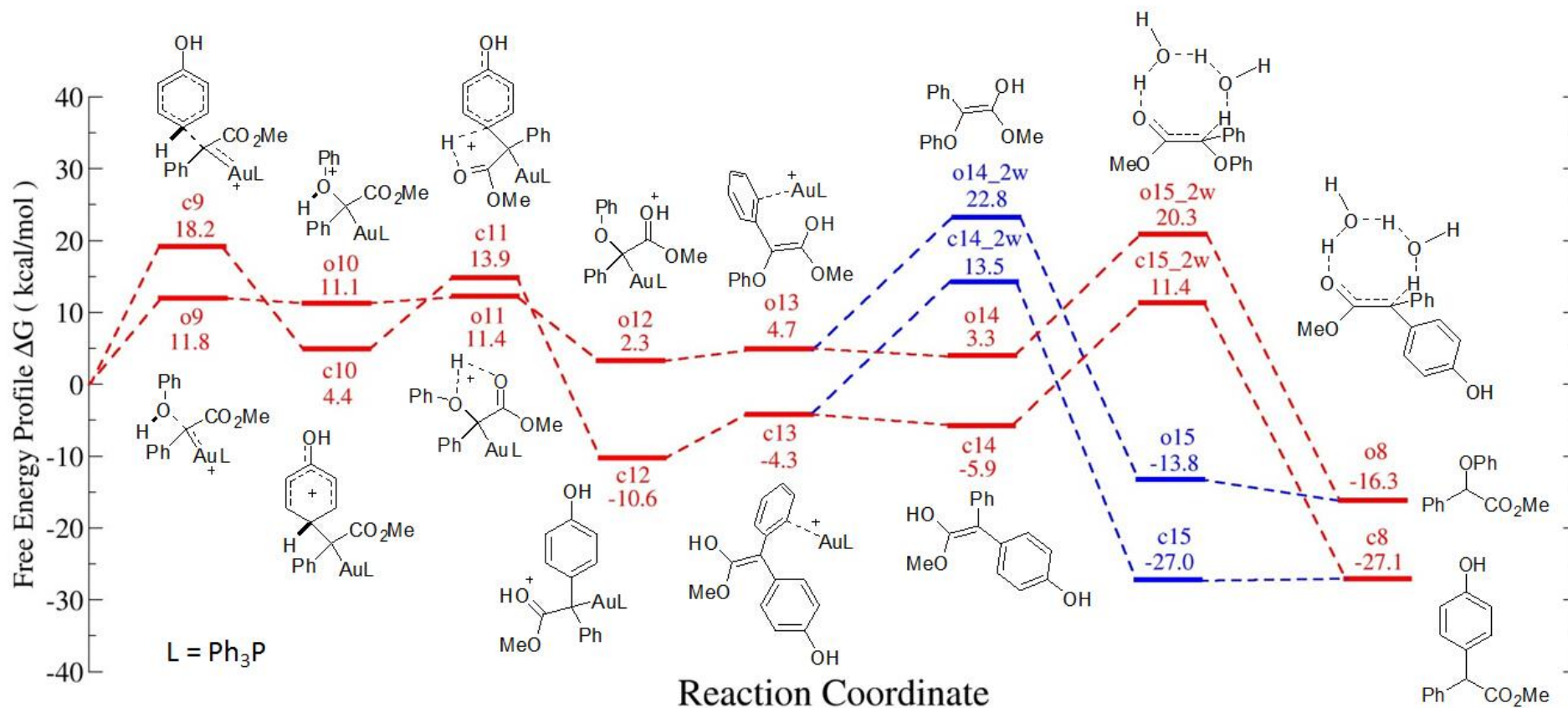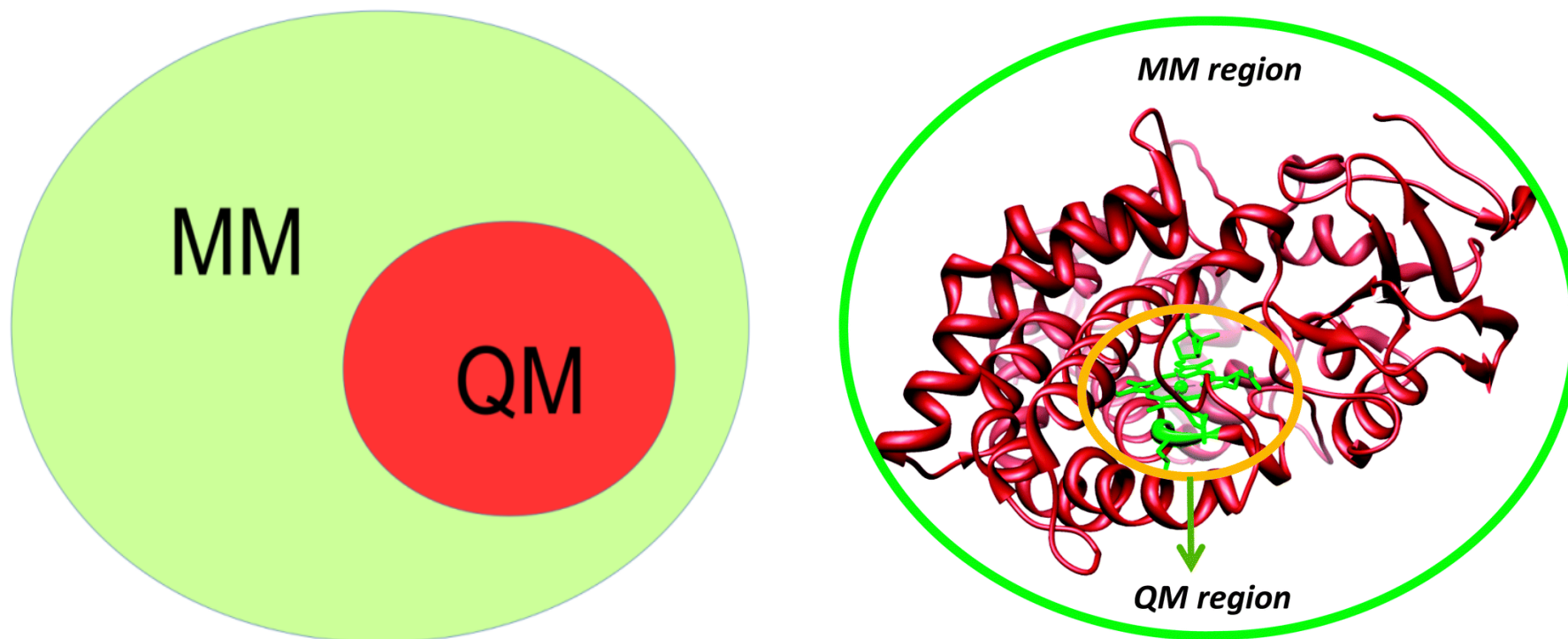


Fei Xia's study

# Transition State and IR Vibrations



Fei Xia's study
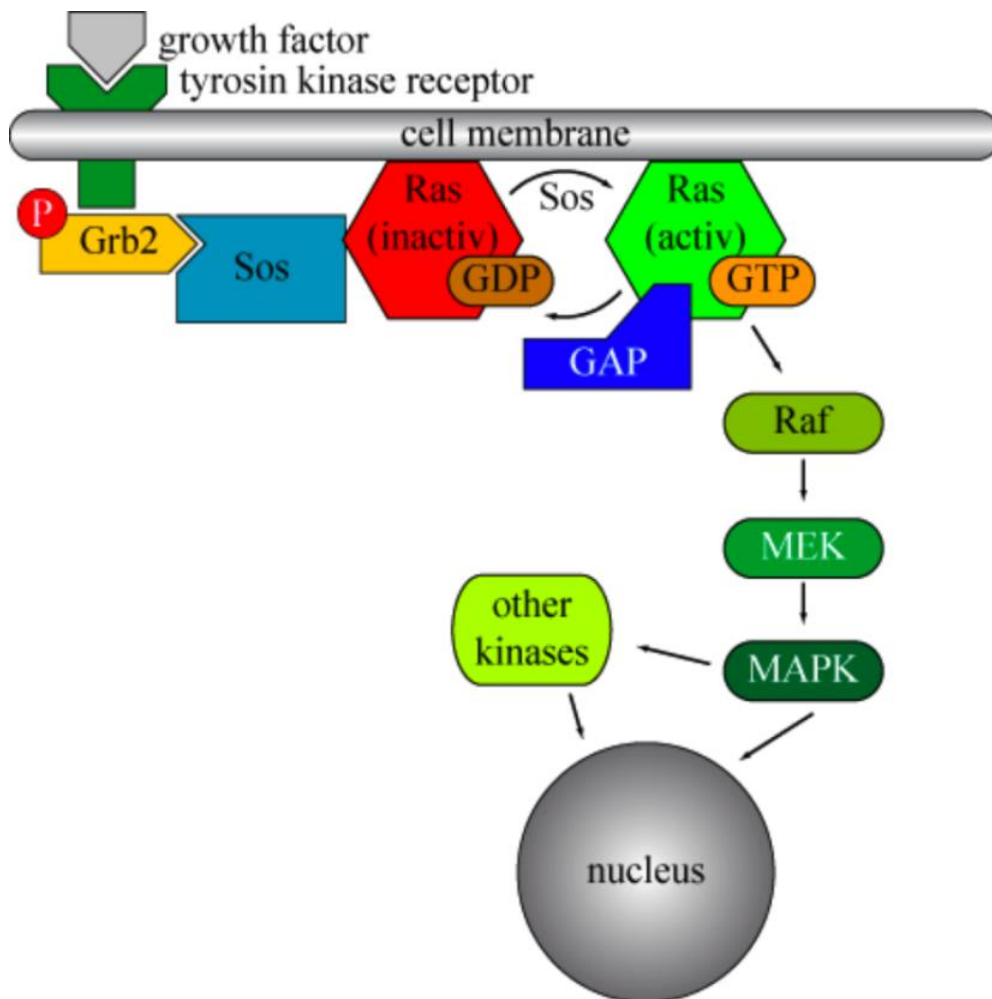
# QM/MM Simulation of Chemical Reactions in Proteins
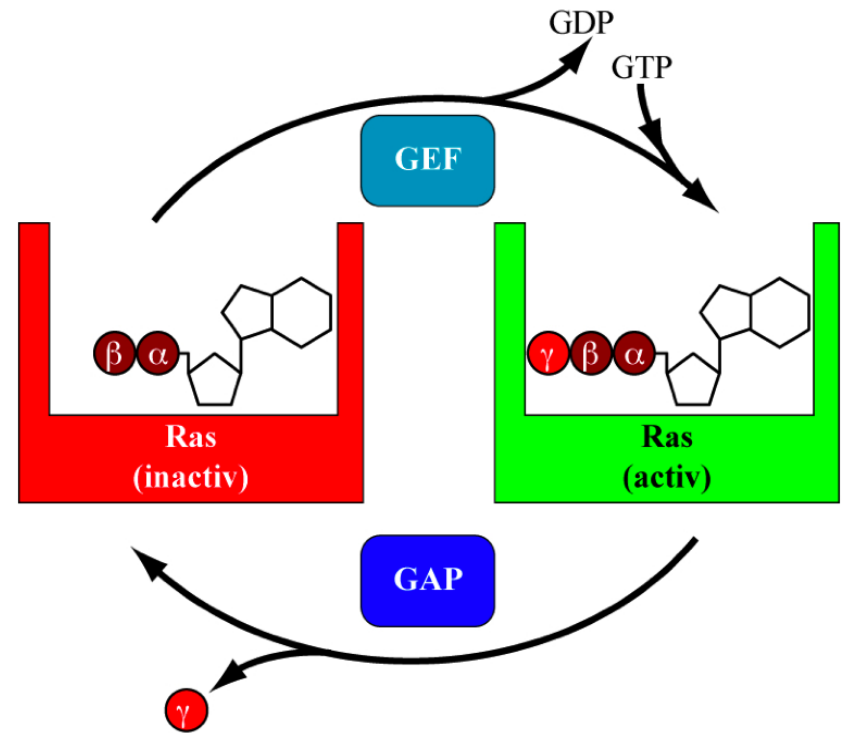


QM: quantum mechanics methods

MM: molecular mechanics methods
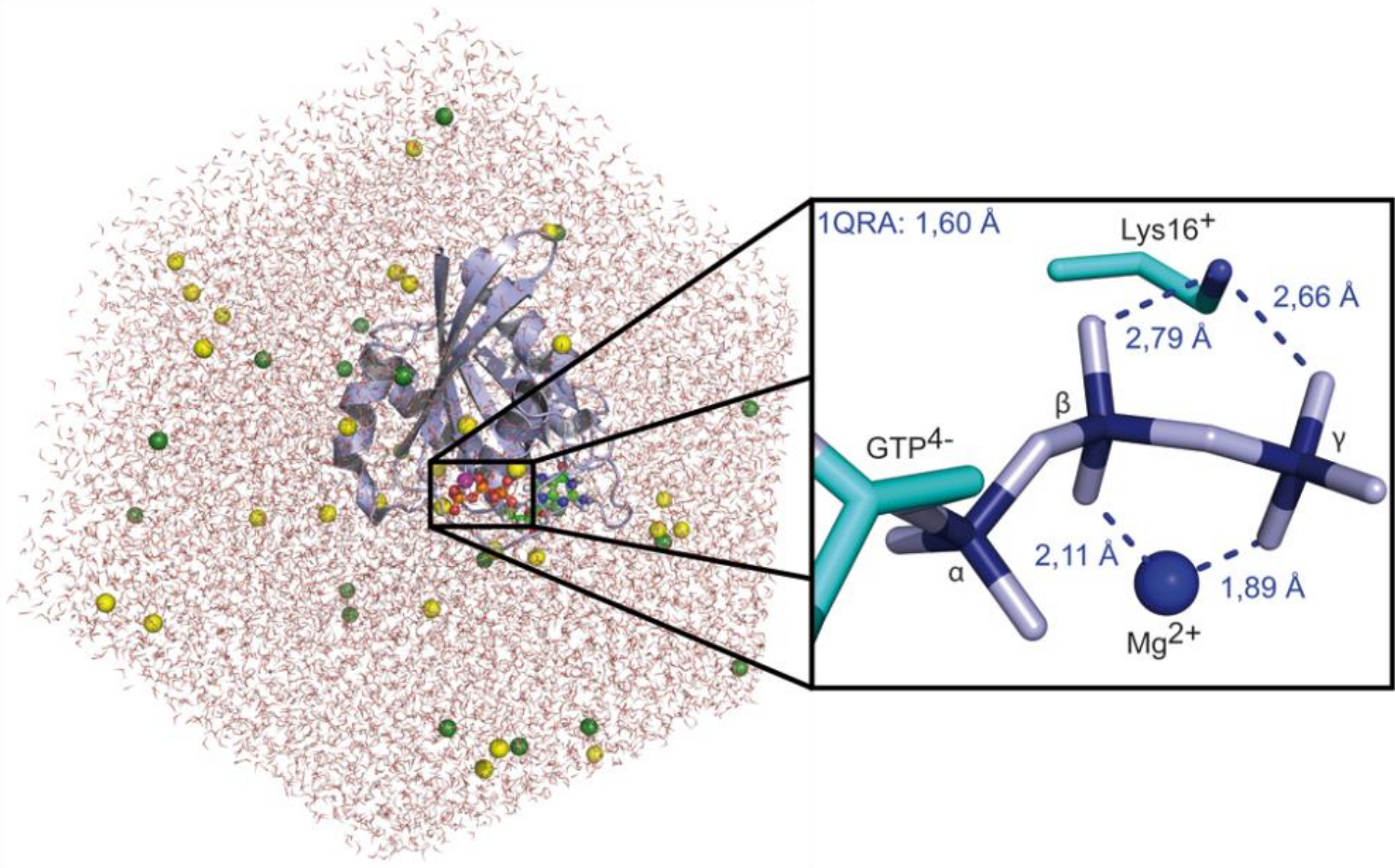
# Function of Ras Protein
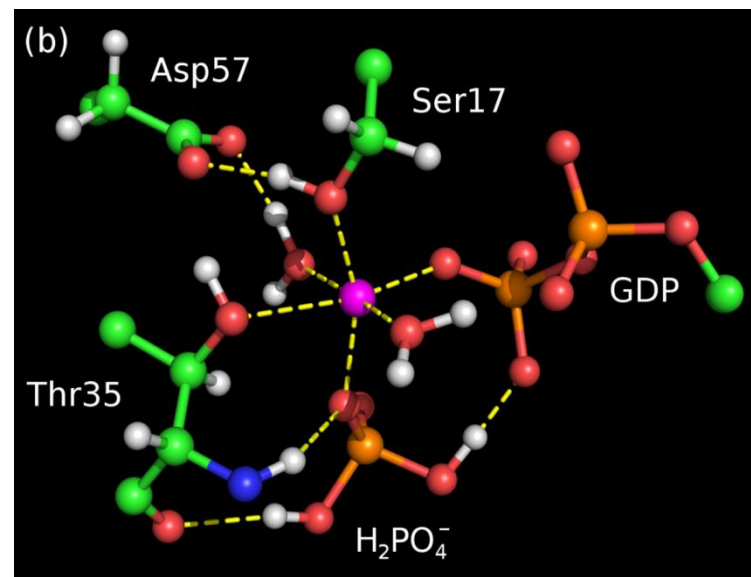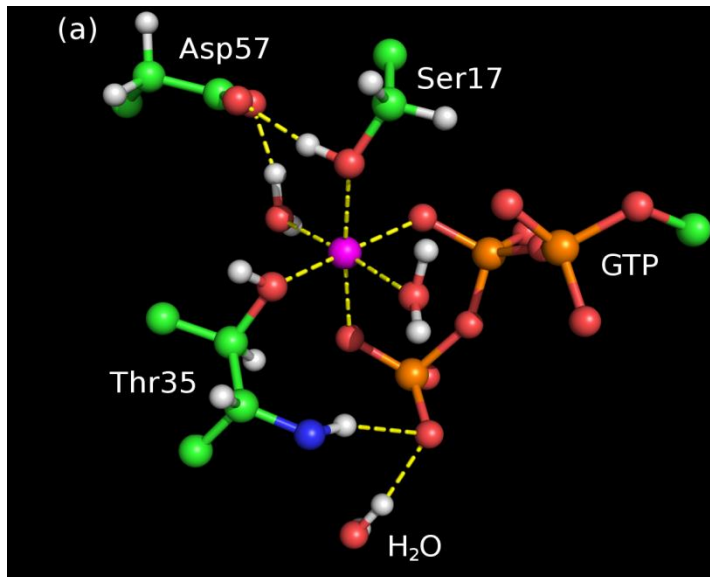
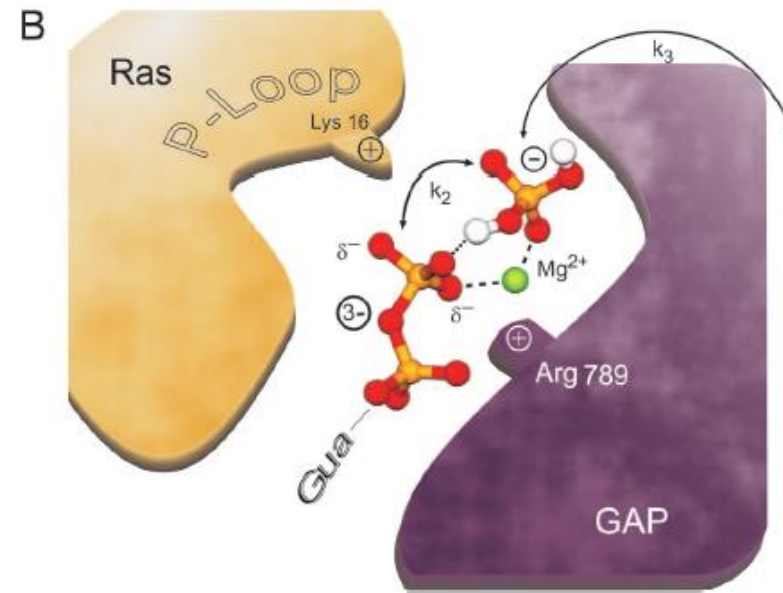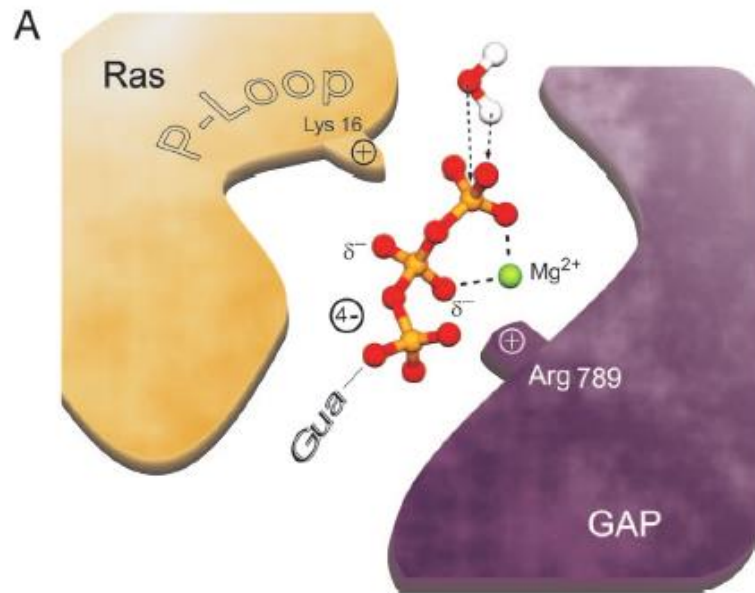## Ras/Raf/MAPK Pathway



## GTP/GDP Cycle



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

# The QM/MM Simulation

# Reaction Mechanism of GTP to GDP

*Thank you for your attentions!*

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