Multiscale Computer Simulations for Chemistry, Biology, Material and Energy Sciences

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Summary of Ongoing GRIDPOINT Projects

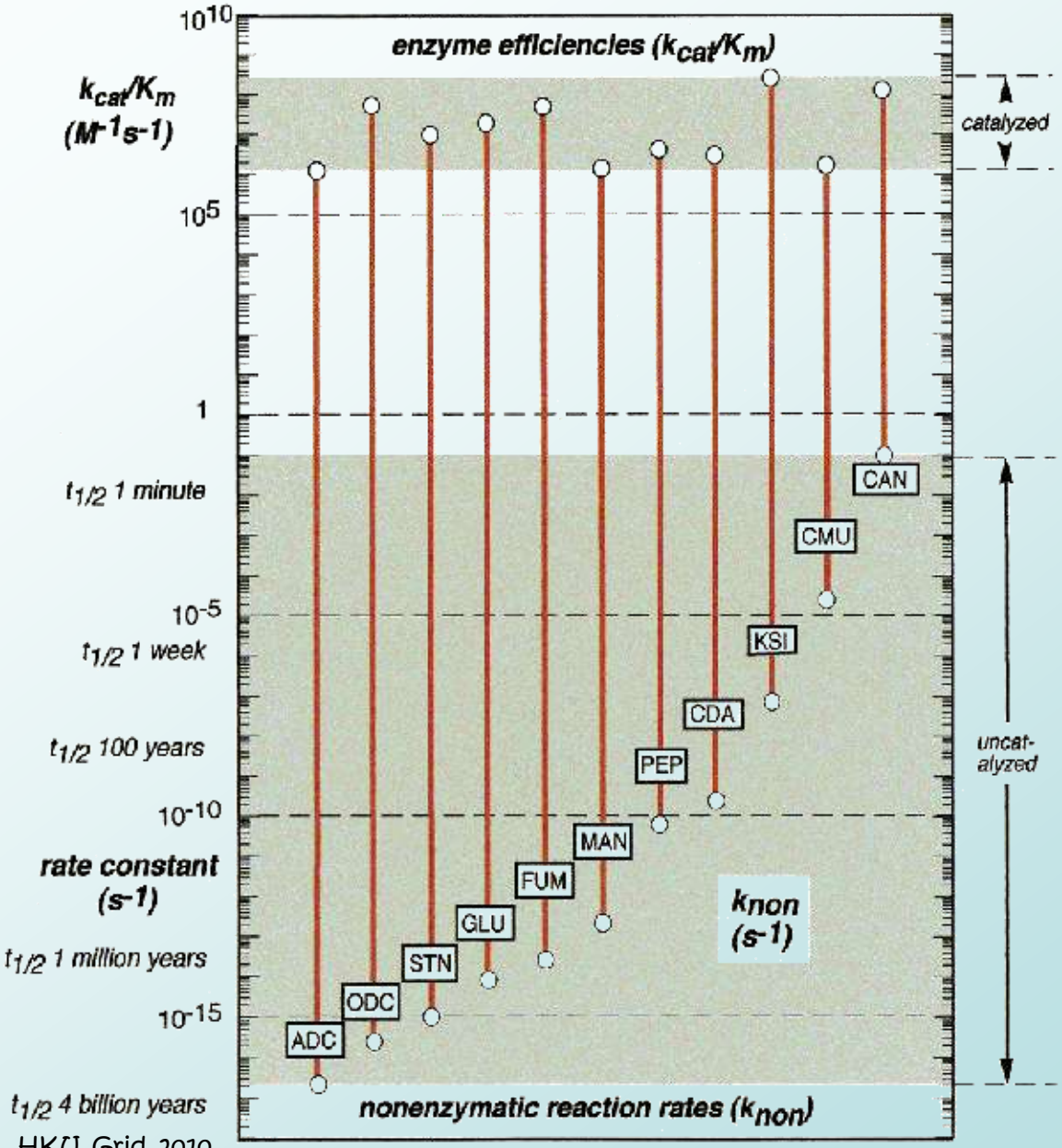
- Dr. H. Hu

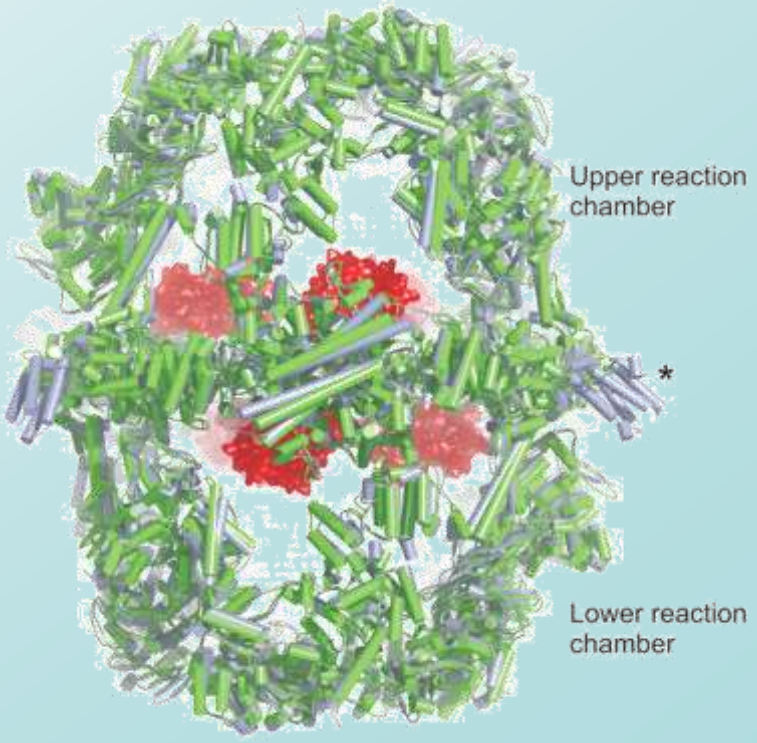
  Computer Simulations of Biomolecular and Chemical Processes for Medicinal and Material Sciences

- Prof. K. Y. Chan

  Computation of Materials & Transport Related to Energy Applications

Enzyme: Extraordinary Catalyst for Life

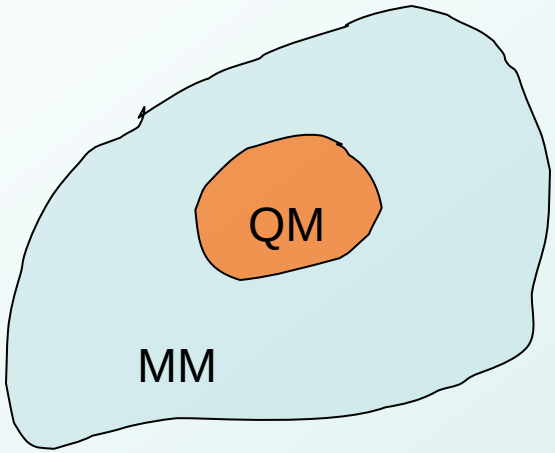




Enzyme: Target for Medicinal and Industrial Research

- Many enzymes are key players in critical physiological processes
  - Target for drug design for cancer research
- Enzyme design for new chemistry
  - New synthesis
  - Energy research

Methodology Developments for Simulating Enzymes



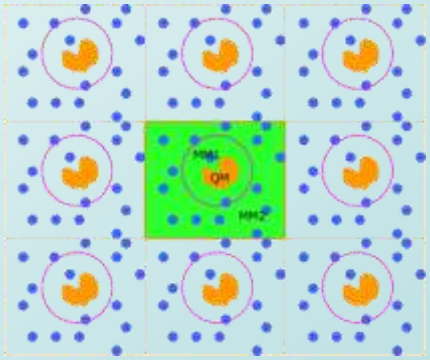
Combined Quantum Mechanical / Molecular Mechanical Method

Technical Challenges

- Speeding up quantum mechanical calculation

$$H\Psi = E\Psi$$

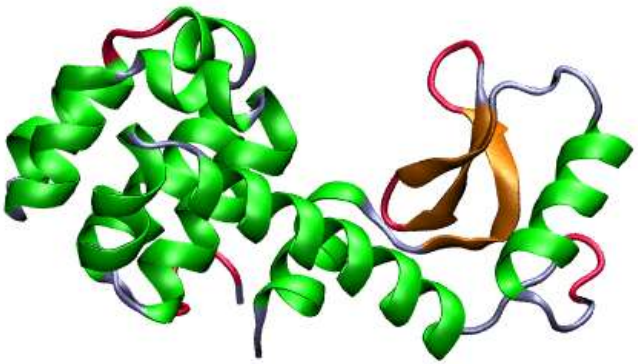
- Proper consideration of long-range forces

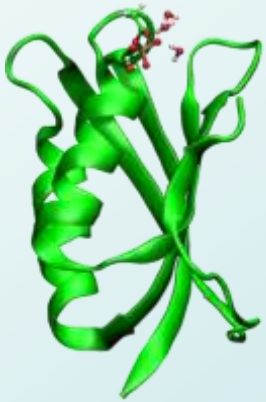


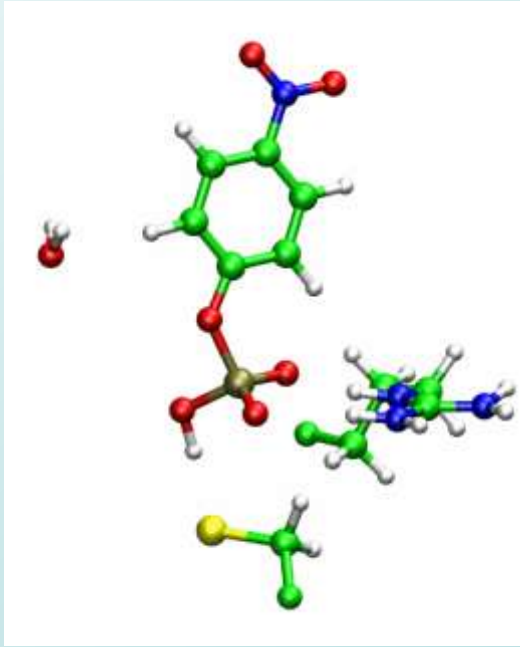
- Sufficient sampling of enzyme conformations

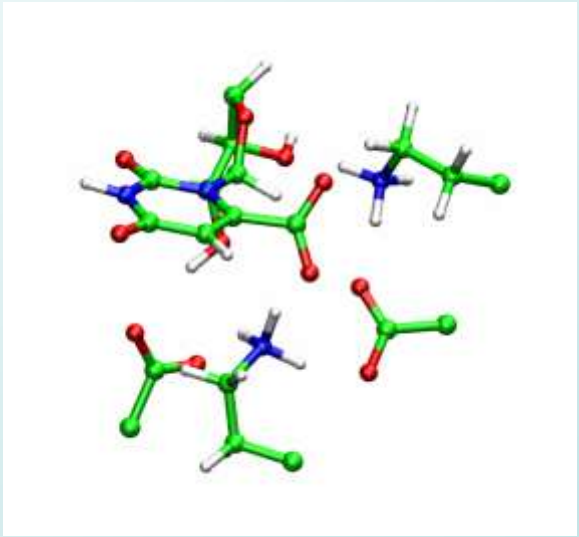
Ultimate goal: Simulate ***bigger*** molecules, at ***longer*** timescale, with ***better*** accuracy

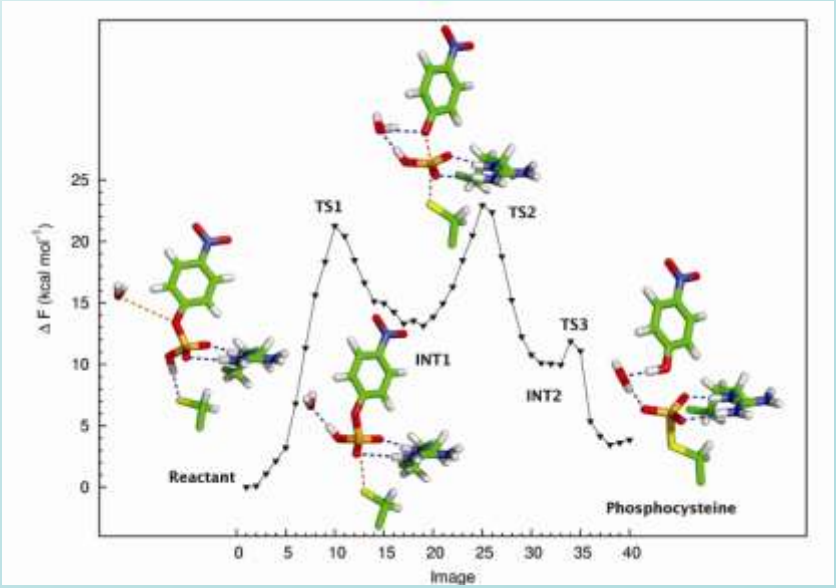
Simulating Enzymes Catalysis



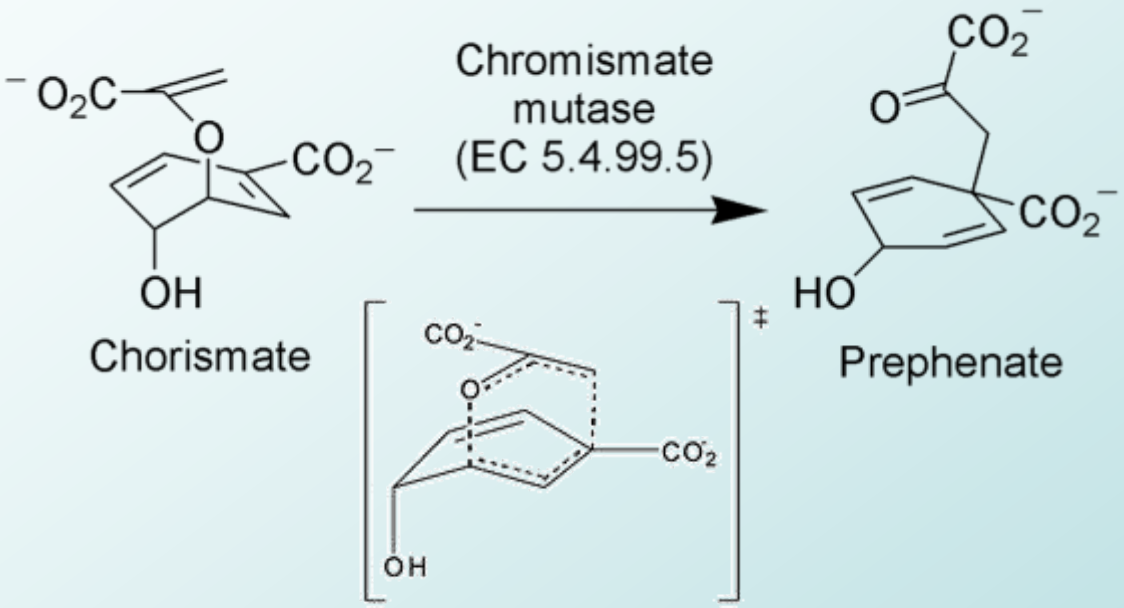


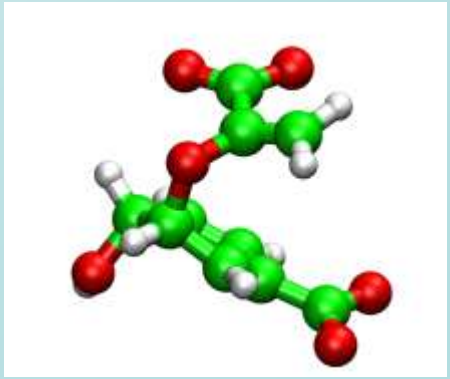






Simulation of Enzyme Catalysis

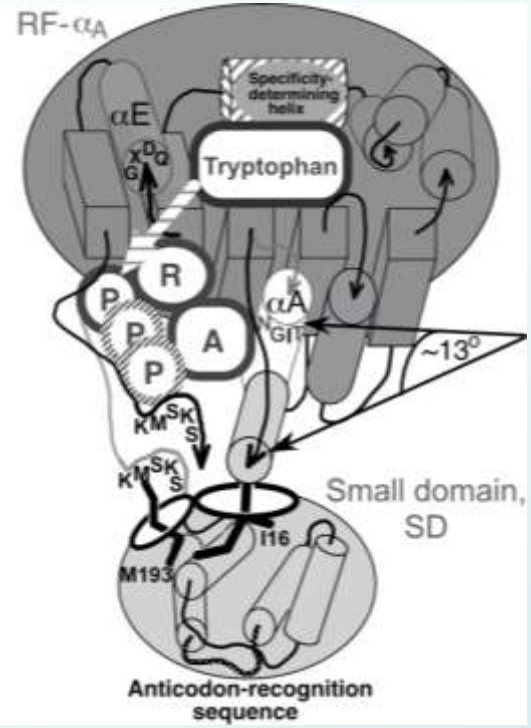


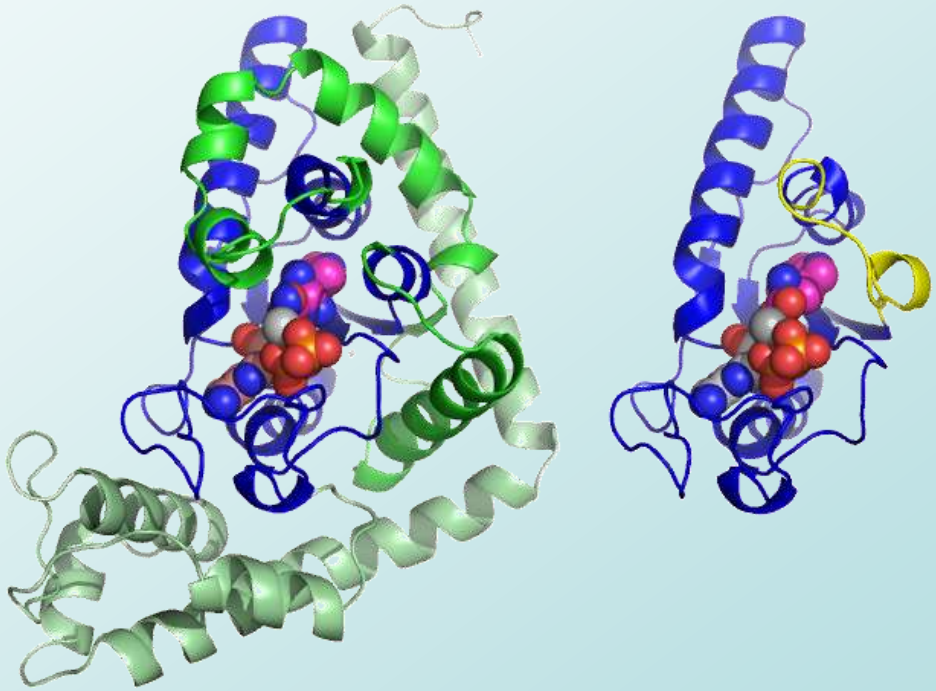


Chorismate mutase

- Synthesis of Phe and Tyr
- Only exists in fungi, bacteria, and higher plant
- Target for fighting Tuberculosis, especially drug-resistant Tuberculosis

Simulation of Enzyme Catalysis





Aminoacyl-tRNA synthetase

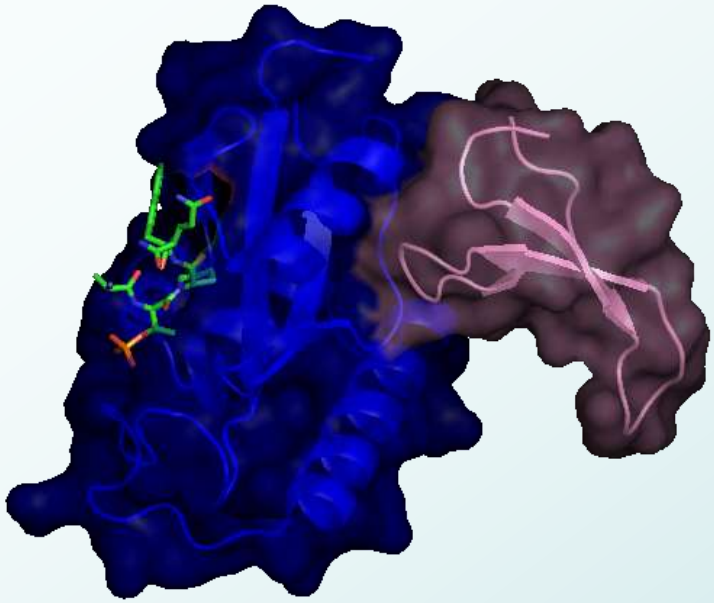
Activation of amino acid

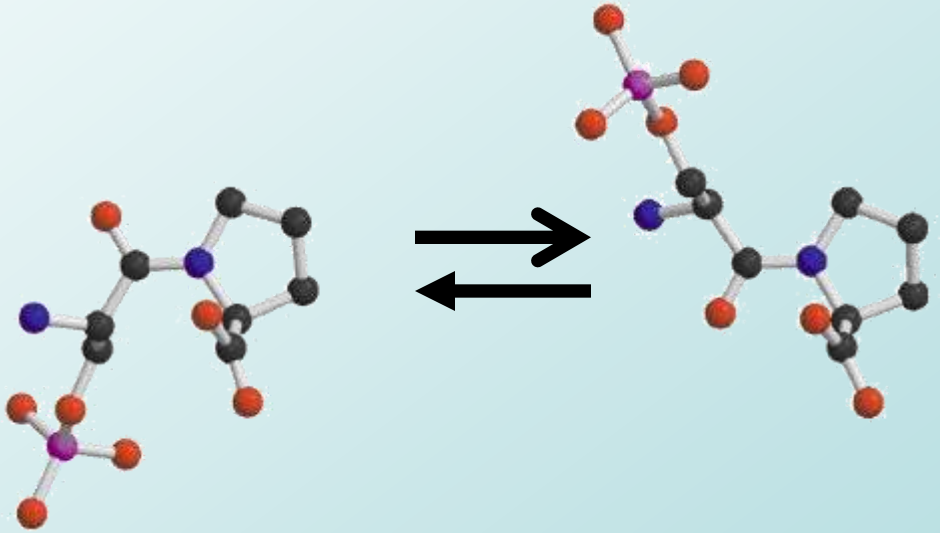
Amino acid + ATP ========> Aminoacyl-5‘AMP + PPi

Reaction mechanism is unclear

Evolution of the enzyme is interesting.

Simulation of Enzyme Catalysis





Pin-1

Catalyzes cis/trans isomerization of peptidyl-prolyl bond.
plays key roles in many important physiological/cellular processes

Other Projects

- New methods for quantum chemistry calculations: linear-scaling
- Enzyme design
- Molecular docking/design for drug discovery
- Multi-scale methods for the structure, dynamics, and recognition of important giant biomolecular complexes

Prof. K.Y. Chan's Research

Computation of Materials & Transport Related to Energy Applications

Multi-Scale Methodology:

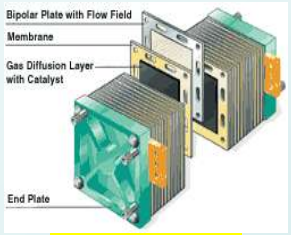
Equilibrium Molecular Dynamics (EMD) Non-Equilibrium Molecular Dynamics (NEMD) Car-Parrinello Molecular Dynamics (CPMD) Monte Carlo (MC), Continuum Mechanics

Collaborator: Dr. David Yu-Hang Chui, now in Melbourne University

System Integrated Devices

HKU Fuel Cell Cart

A DMFC powered cellular phone

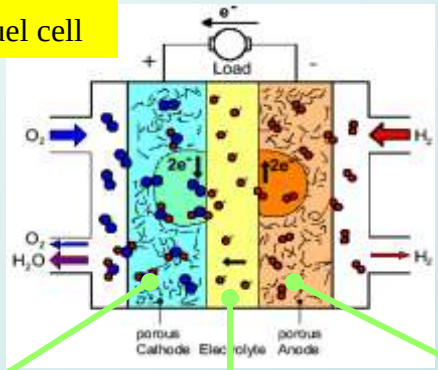


fuel cell stack

HKU made

Macroscopic Structuring

A single fuel cell



Cathode Electrode:
$½O_2 + 2H^+ + 2e^- \rightarrow H_2O$

Oxidant

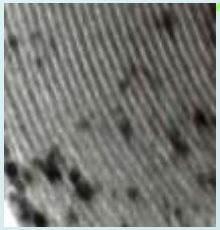
Anode Electrode
$H_2 \rightarrow 2H^+ + 2e^-$

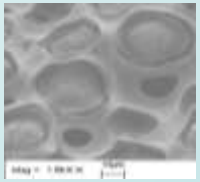
Fuel

alcohols
glucose
Liq. fuels
$\rightarrow CO_2 + H^+ + 2e^-$

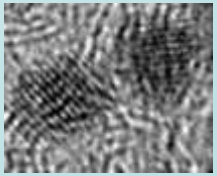
Nanoscopic

Nano Size dependence catalytic activity





cationic, anionic, bipolar nano polymeric-ceramic membranes



TEM Image of Nano Catalyst

Mixed Nano Metal/Metal Oxides: Pt/Ru/Co/Sn/W Mesoporous carbon

Molecular/ Atomic

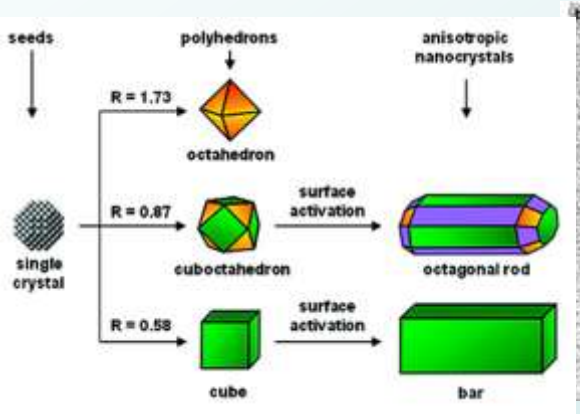
Cu, Fe, Pt, support

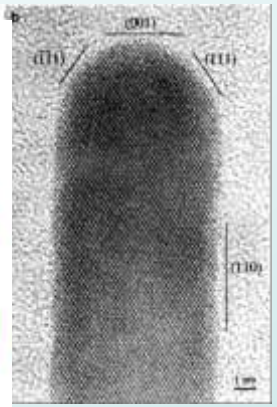
Bottom up research strategy

Computing / Modeling ↔ Synthesis ↔ Properties

Nanostructuring of metals

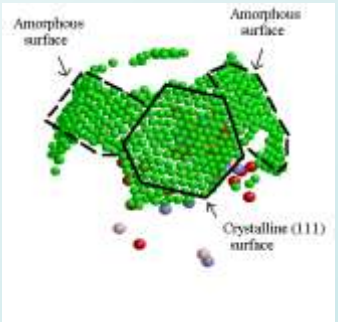
Problem

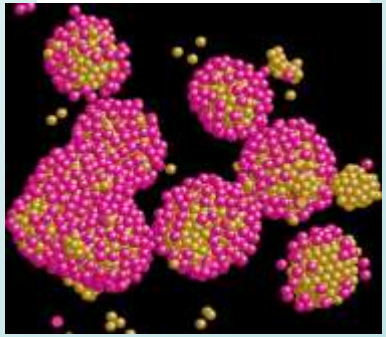


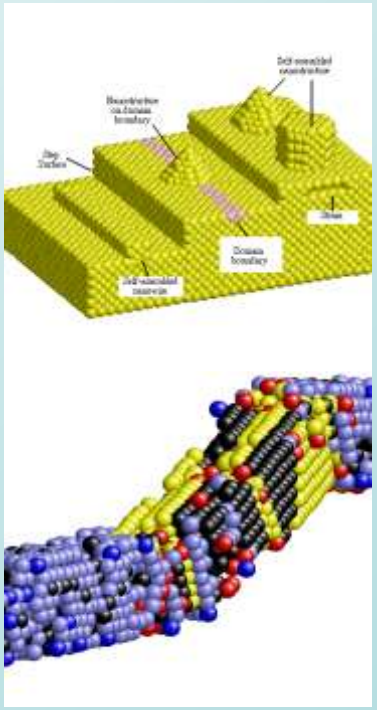


Limitations in characterization lead to poor understanding of nanostructures

Tools







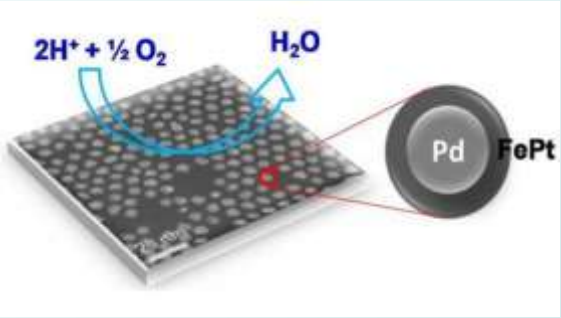
Simulations and modelling help to understand the formation and properties of nanostructures

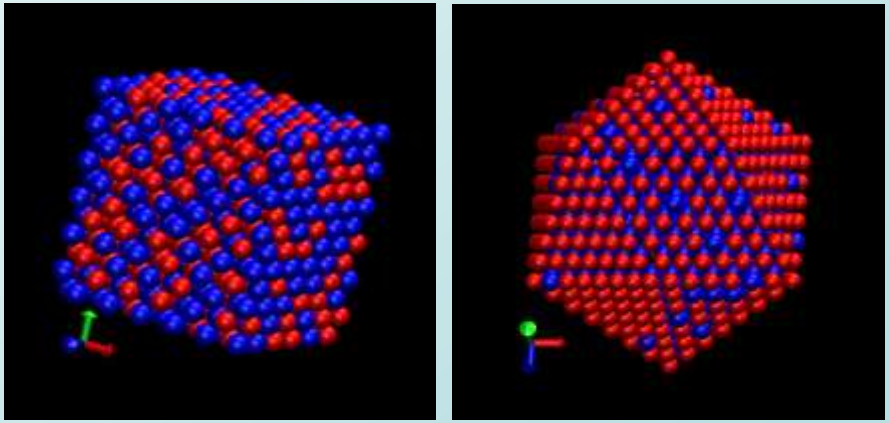
Chui and co-workers, 2004-now

Modelling core-shell Mixed Metal nanoparticles at HKU

Combine classical and quantum calculations to investigate the effect of shapes, sizes, and compositions
on the catalytic activity of nanoparticles.

to design a durable and more efficient nano-catalyst for fuel cell applications.





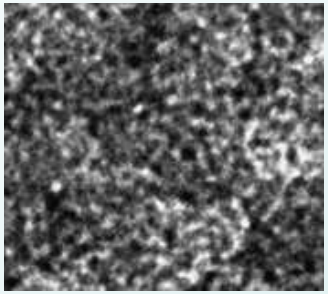
Red - Pt Blue - Cu

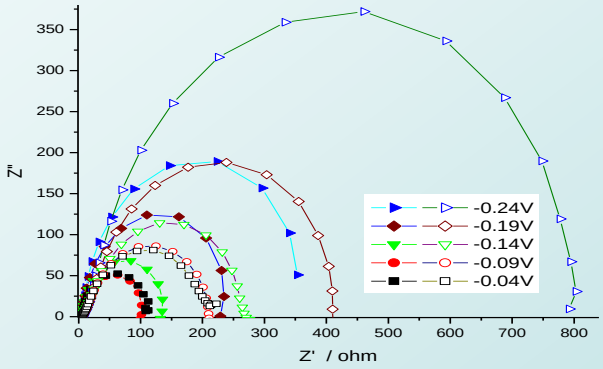
Observed phase change in core/shell PtCu/Pt nanoparticles
Understand lattice strain control in core-shell structures.
The computational time : 2 hours on HKU Gridpoint

Ionic Transport in Nanopores

Experiments

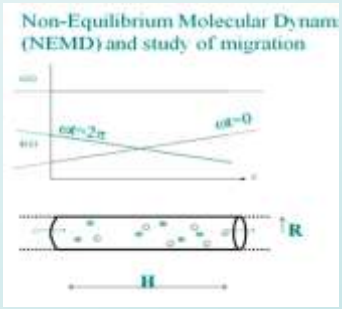
AC Impedance in Nanoporous Electrodes



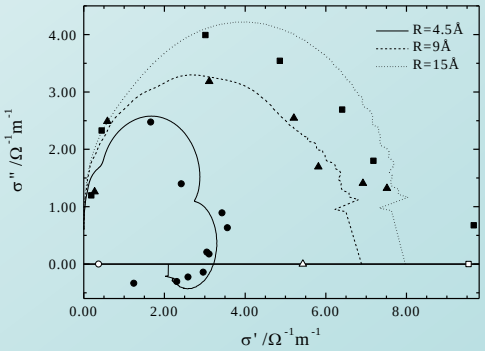


Ren, Ding, Chan, & Wang, *Chem Mater*

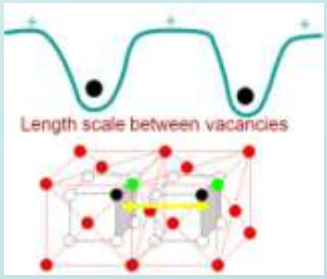
NEMD Simulations with AC Electric Field applied



SPC/E Electrolyte



Tang, Szalai & Chan, *Nano Letters*



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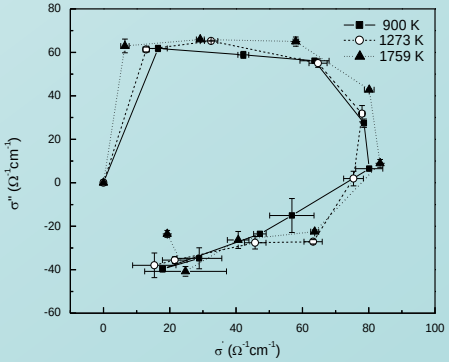
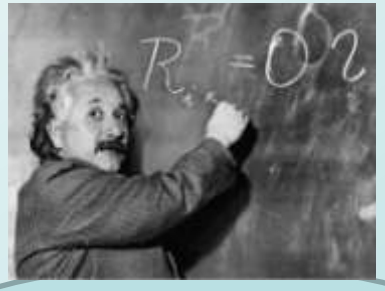


Zhang & Chan, *J. Phys Chem*

The (Old) Ecologic System for Academic Research



Theory

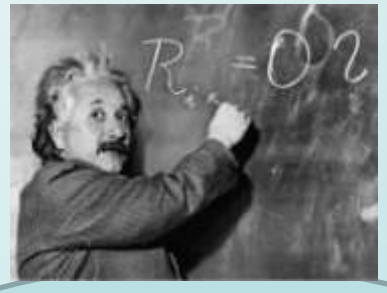
Experiment

Industry

Money

The (New) Ecologic System for Academic Research

Experiment



Theory

Industry

Money

Simulation & Modeling

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Thank You