Understanding and designing materials and processes via computational chemistry and engineering

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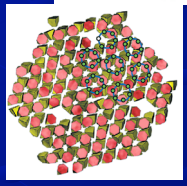
The Chemical Engineering Profession

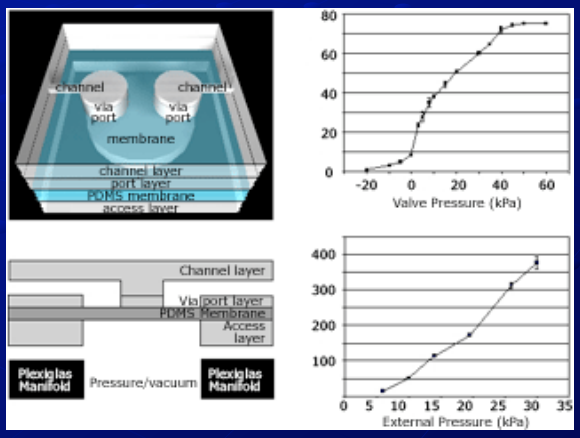
This is traditional Chemical Engineering….

New focus

- From chemical processes to chemical products:



nanotechnology



Lab on a chip

Molecular level knowledge

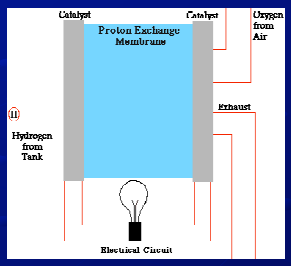
New chemical engineering designs require reaching the atomistic world

How?
Solving exact laws of nature

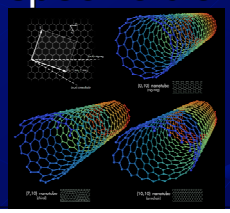
Numerical solutions involving realistic models now possible because of supercomputers

Examples of our research

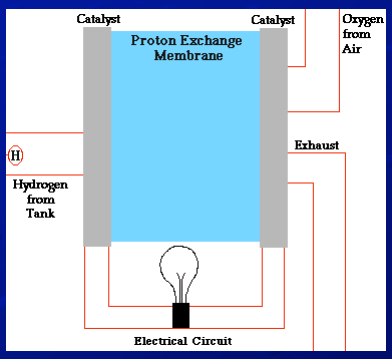
- Design of new catalysts for alternative power sources



- Design of catalysts for fabrication of carbon nanotubes with specific diameter and chiralities



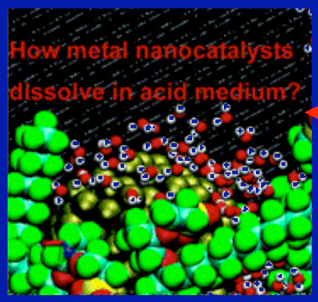
Fuel cell converts chemical energy into electricity



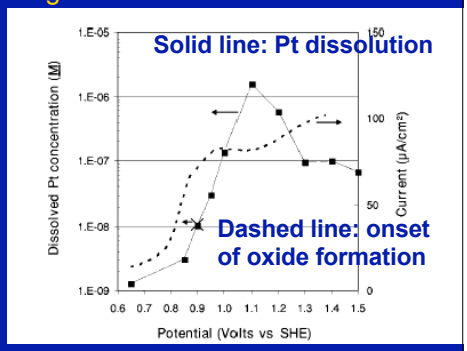
Challenge: **Catalyst design**
Platinum best catalyst, scarce and expensive!!!
Computational design of alternative materials already helping

Fuel cell nanocatalysts durability: how theory and simulation can help

P. B. Balbuena et al, Texas A&M



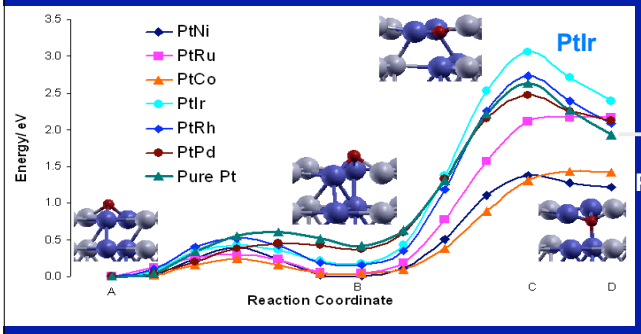
Because of the nanosize of the catalyst:
- activity is a function of particle size, shape
- enhanced effects of particle-substrate interactions
- **dissolution of metal atoms in acid medium**
- particle sintering



Our DFT studies suggest that:
1) Formation of a surface oxide film is the initial stage of metal dissolution
2) Alloys may shift the onset of oxide formation to more positive potentials

Experimental results: **Wang, Kumar, Myers, ESSL, 2006**

DFT studies show that certain Pt-based alloys have higher barriers for penetration of oxygen into the subsurface



PtIr

PtRh

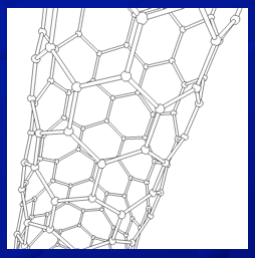
Pt (111)

Pt Co, PtNi

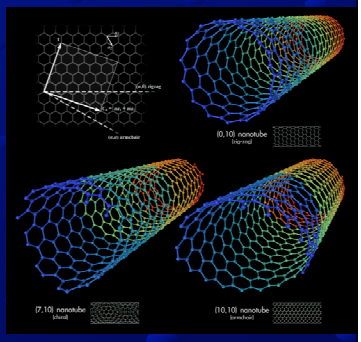
DFT calculated barriers for oxygen diffusion on the surface (left) and migration into the subsurface (right)

- **Pt-skin surfaces show better stability against dissolution than pure Pt surfaces**
- **A shift to more positive potentials is predicted for the onset of oxide growth for specific alloy compositions**
- **A clear correlation is established between alloy composition and stability**
- **Results of the surface segregation process (key for alloys) are obtained under reaction conditions**

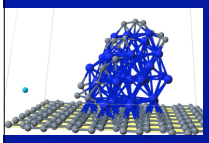
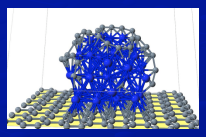
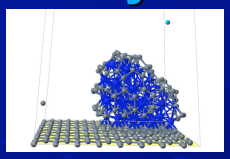
Design of catalysts for fabrication of single-wall carbon nanotubes



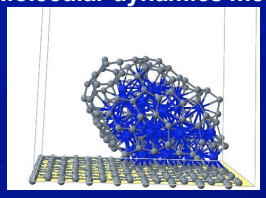
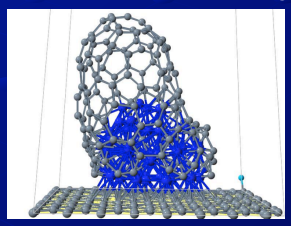
Potential applications:
Medicine
Desalinization of water
Optical and electronic devices



Single-wall carbon nanotubes grow over catalysts

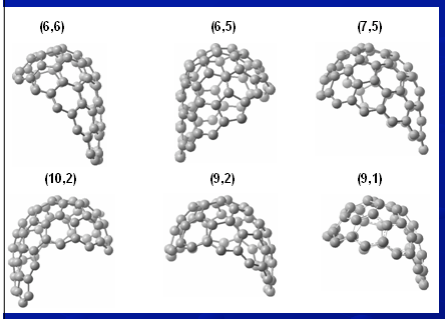




Images show simulated growth process over cobalt nanoparticles. Molecular dynamics methods were implemented by our group.

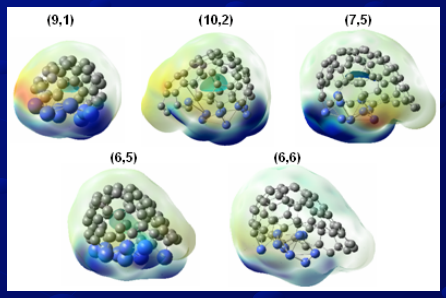



Challenge: Is it possible to produce tubes with specific diameters and chiralities?

Initial stages of growth

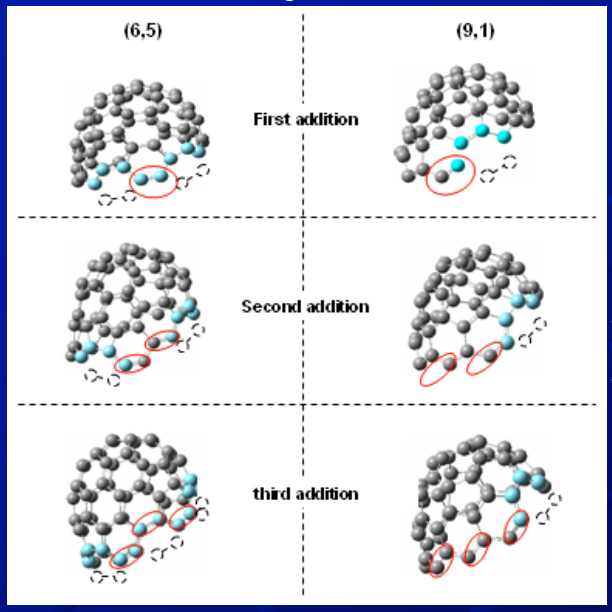


What defines the nanotube chirality during growth?



Interactions cluster-nascent cap, Role of catalyst shape, size, chemical composition, elucidated via first-principles calculations

Differences in rates of growth determined computationally



Goal:

Understanding chemistry of growth process will lead to a controlled design of the fabrication process

Summary

- Computational work yields firm guidelines for catalyst design
- Collaborators:
  - DOE supported grant for fuel cell catalysts is a multi-institutional project TAMU-United Technologies Company-Johnson Matthey Co.-Brookhaven National Lab
  - DOE supported project for carbon nanotubes is in collaboration with Prof. Resasco from Southwest Nanotechnologies, Oklahoma

Acknowledgments

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- Department of Energy/Basic Energy Sciences for financial support

Thanks for your attention !!!