Computational Catalysis and Electrocatalysis

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SC Annual User Meeting 2009, 20th Anniversary Celebration, May 6th, 2009

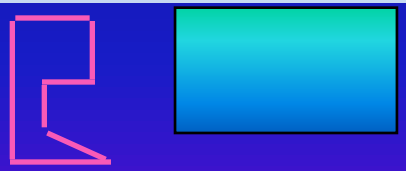
Why catalysis?

Most Reactions are too slow to be useful...

Catalyst-Reactants

Catalyst + Reactants

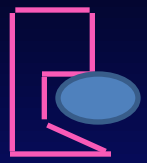
Catalyst + Products



Catalysts speed up a chemical reaction

without being used up...

Why computational catalysis?



????

A good catalyst is a material whose surface is composed of active sites where reactants may be temporarily attached or may be decomposed

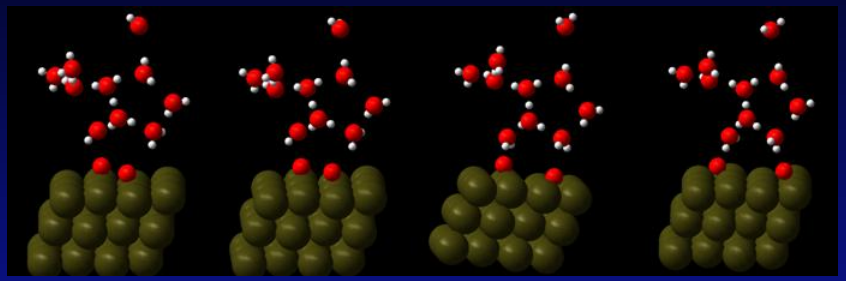
The challenge: find out an efficient, durable, and cost effective materials for catalysis

Experiments help, but… Too lengthy and expensive !!!

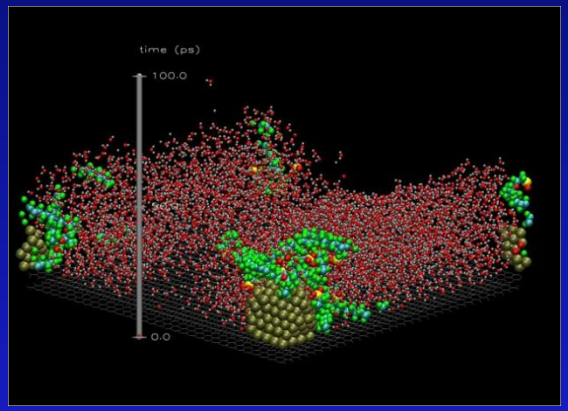
First-principles based computations are excellent tools to guide experiments and design novel materials

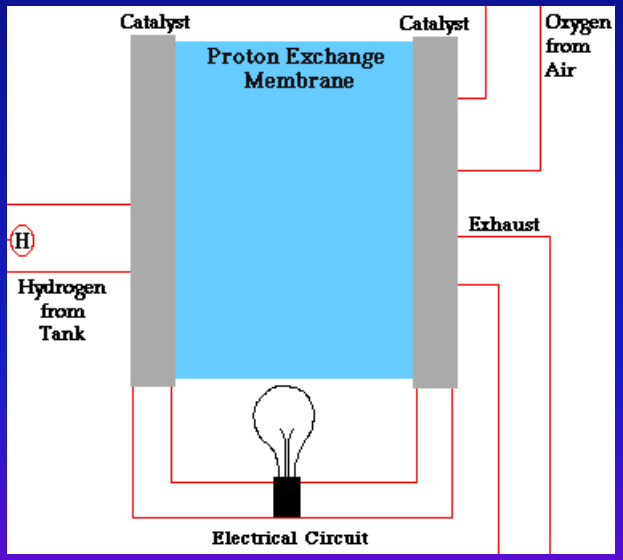
Tools-methods

From the atomistic level…



To mesoscopic





And macroscopic systems…

Covering large time scales:
from femtoseconds to minutes, hours…

Tools-hardware

Novel catalytic designs require reaching the atomistic world

How?
Solving exact laws of nature

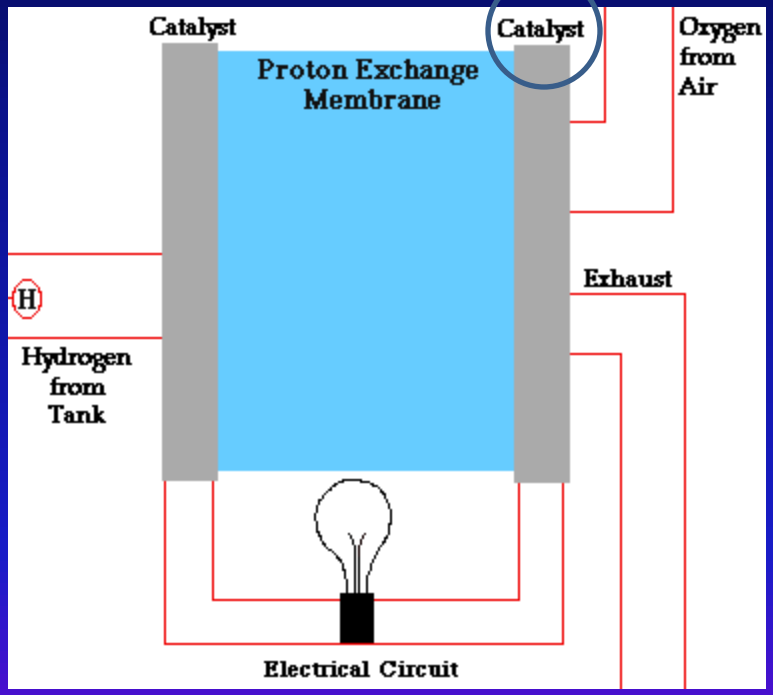
Numerical solutions involving realistic models now possible because of supercomputers

Applications from our research

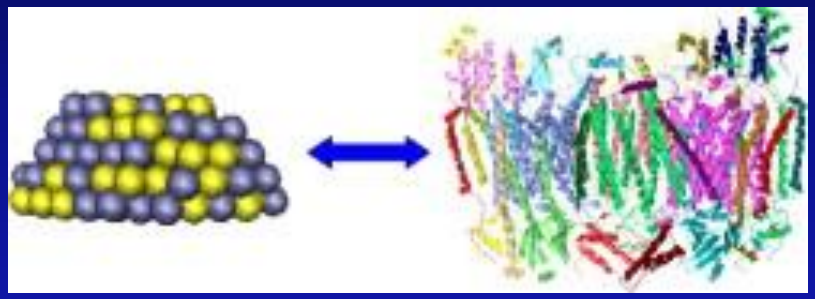
- Fuel cell electrocatalysts
- Controlled growth of carbon nanostructures
- Hydrogen storage
- Photocatalysis

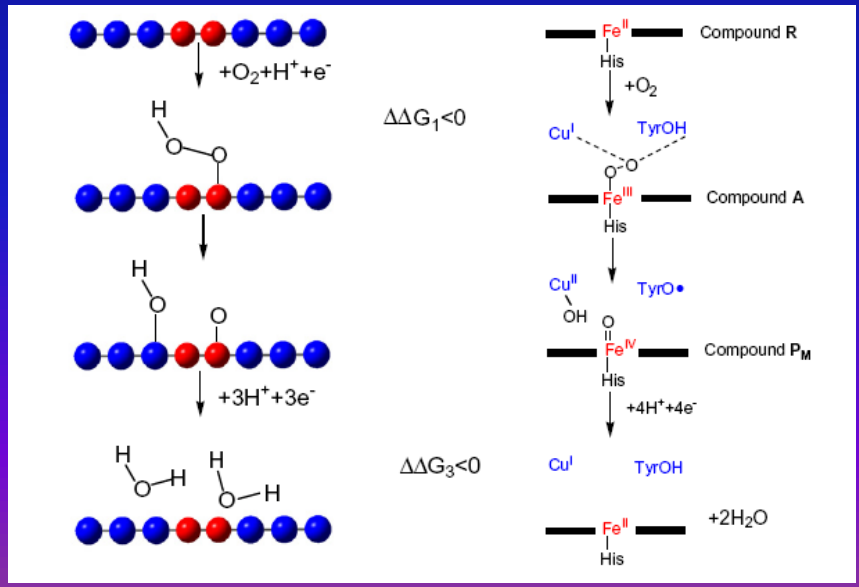
Fuel cell electrocatalysts

Chemical energy is converted into electrical energy



Parallelism between bimetallics and metalloenzymes

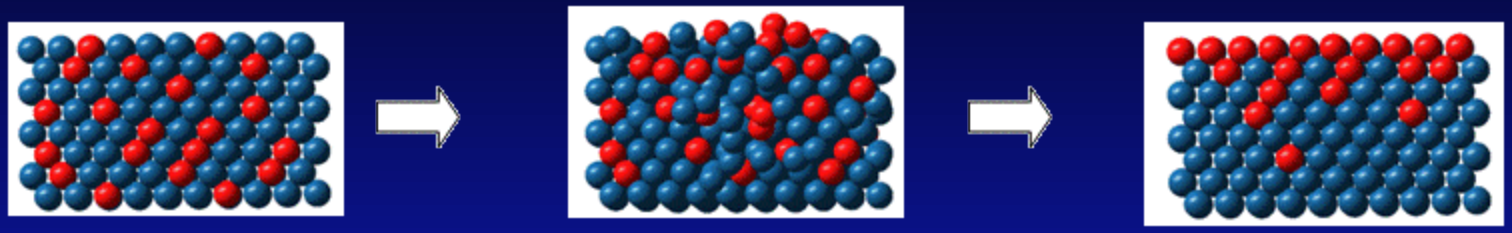




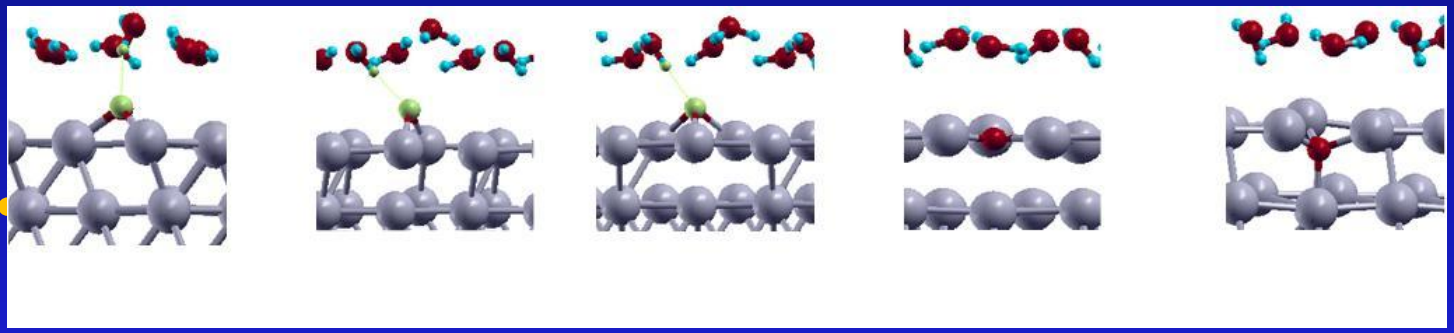
Wang and Balbuena, JPCB 2005;
Ma and Balbuena, CPL, 2007

Predictions and challenges

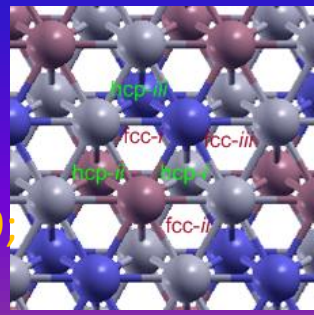
- catalyst surface evolution during reaction



- catalyst degradation in acid medium



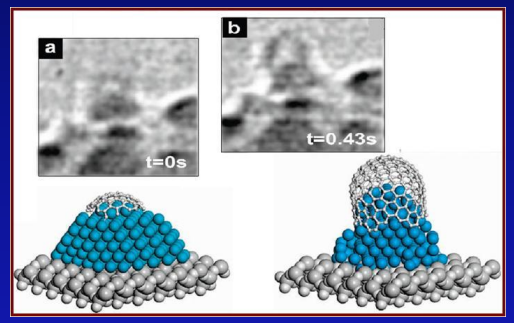
- new formulations of binary and ternary alloys



Ma and Balbuena, Surf. Sci, 2008; Ma and Balbuena, JPCC, 2008;
Ramirez-Caballero and Balbuena, CPL, 2008;
Callejas-Tovar and Balbuena, Surf. Sci, 2008; Hirunsit and Balbuena, Surf. Sci. 2009;
Martinez de La Hoz, Callejas-Tovar, and Balbuena, Mol. Sim., 2009

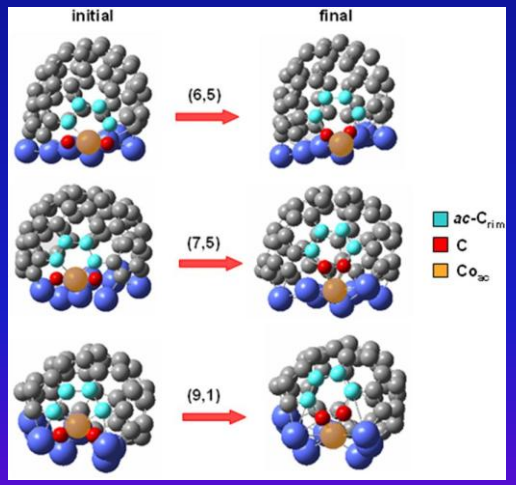
Controlled growth of carbon structures

Carbon structures (e.g. carbon nanotubes) grow over metal nanocatalysts at high temperatures



Robertson et al, Nanoletters, 2007

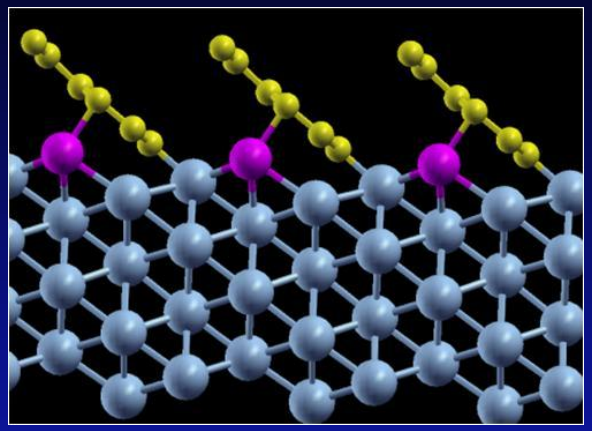
But a controlled growth is desired to form structures with specific properties

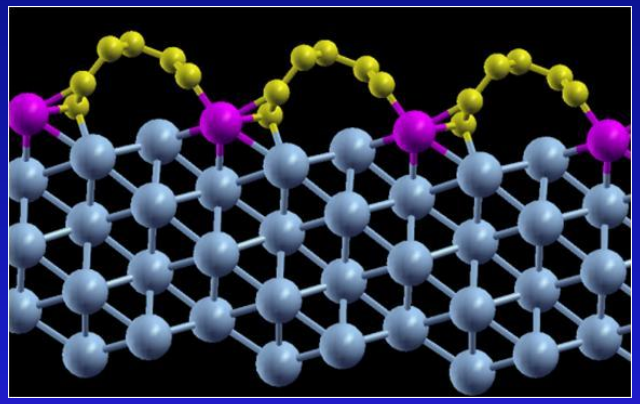


D. A. Gómez-Gualdrón and P. B. Balbuena, Nanotechnology, 2009

Predictions and challenges

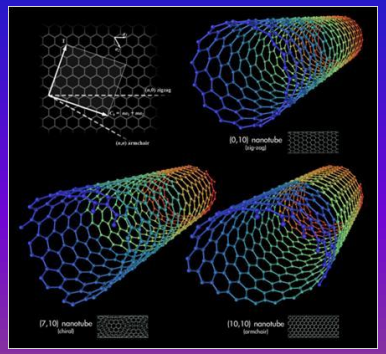
Graphene growth parallel to the (100) plane of Co





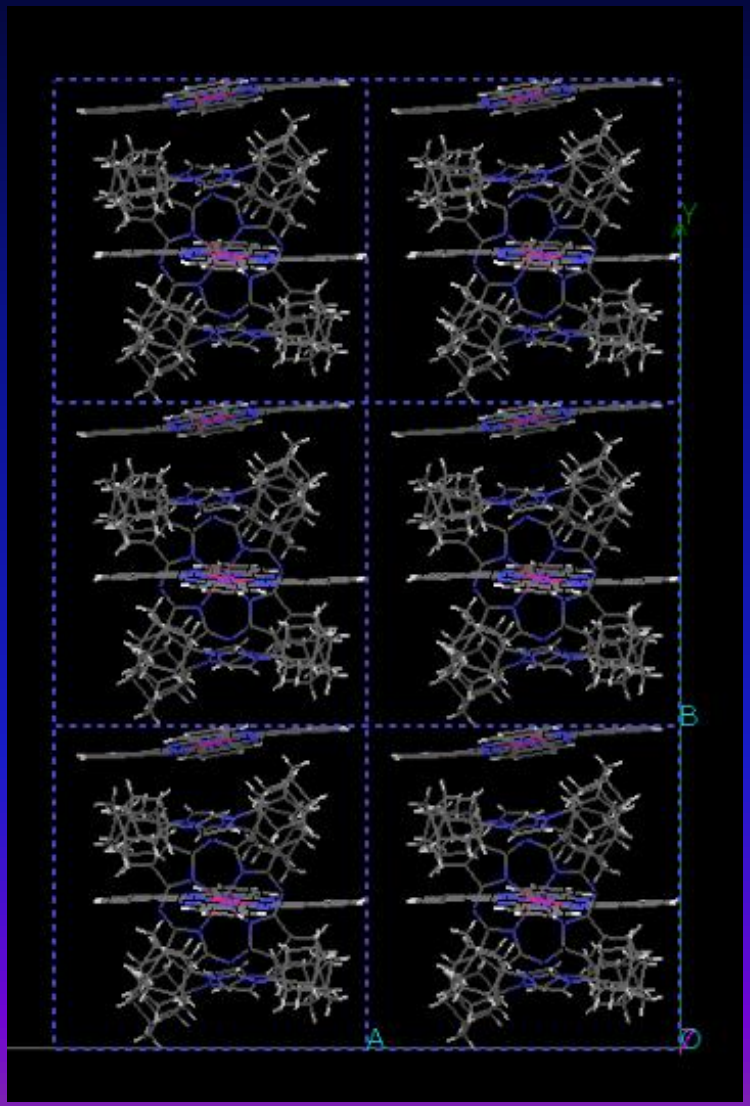
Formation of horizontally aligned semi-nanotubes

G. E. Ramirez-Caballero, J. C. Burgos, and P. B. Balbuena
J. Phys. Chem. C (2009)



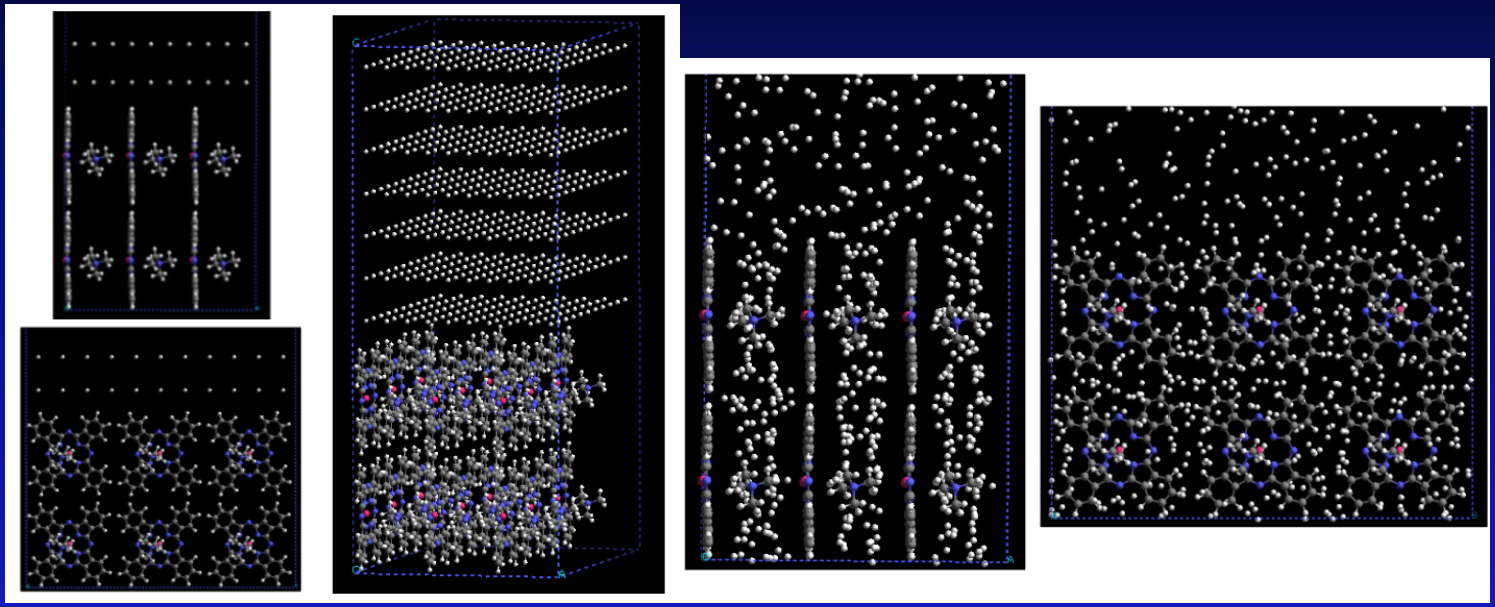
We are working towards predicting controlled nanotube helicity

New materials for hydrogen storage



We are testing new materials that promise good ability for hydrogen storage—Another fuel cell challenge

Predictions and challenges



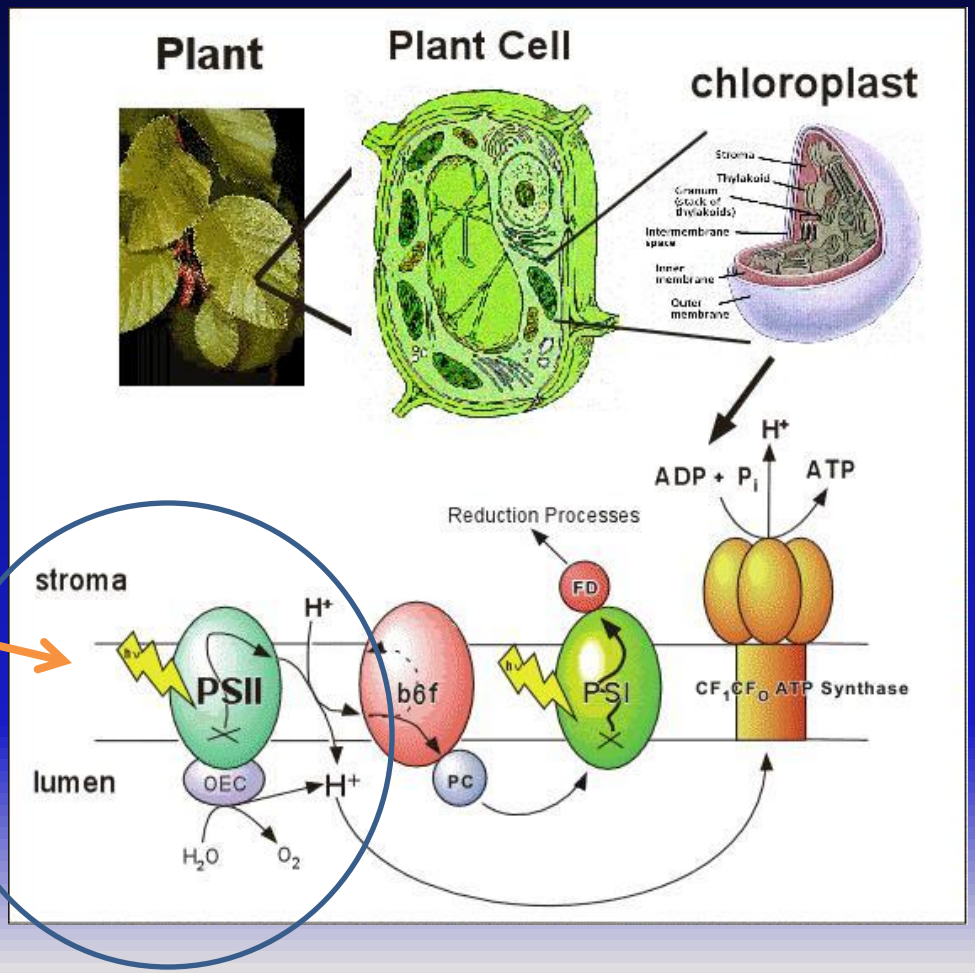
Using molecular dynamics simulations we showed that certain layered materials have good storage capacity at moderate pressures and room temperature

Lamonte, Gomez-Gualdron, Cabrales-Navarro, Scanlon, Sandi, Feld, and Balbuena,
J. Phys. Chem. B, 2008

Future projects: photo-catalysis

Computational studies will be oriented to find new light-harvesting molecules and new catalysts for this important reaction

Photo-catalytic process



water decomposes over a catalyst producing oxygen and hydrogen

From members.tripod.com/beckysroom/pictures2.htm

Acknowledgements

Department of Energy/Basic Energy Sciences for financial support; grants DE-FG02-05ER15729; DE-FG02-06ER15836 and DE-FG36-07GO17019

Special thanks to

TEXAS A&M UNIVERSITY SUPERCOMPUTING FACILITY

SC time from NERSC, ARL, and TACC is also acknowledged