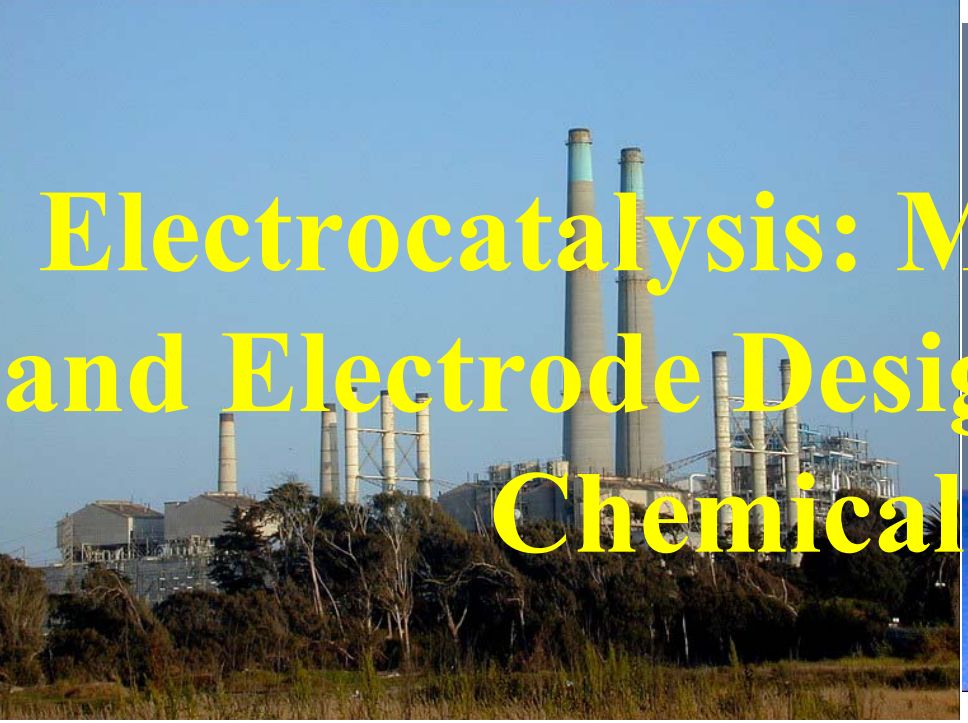
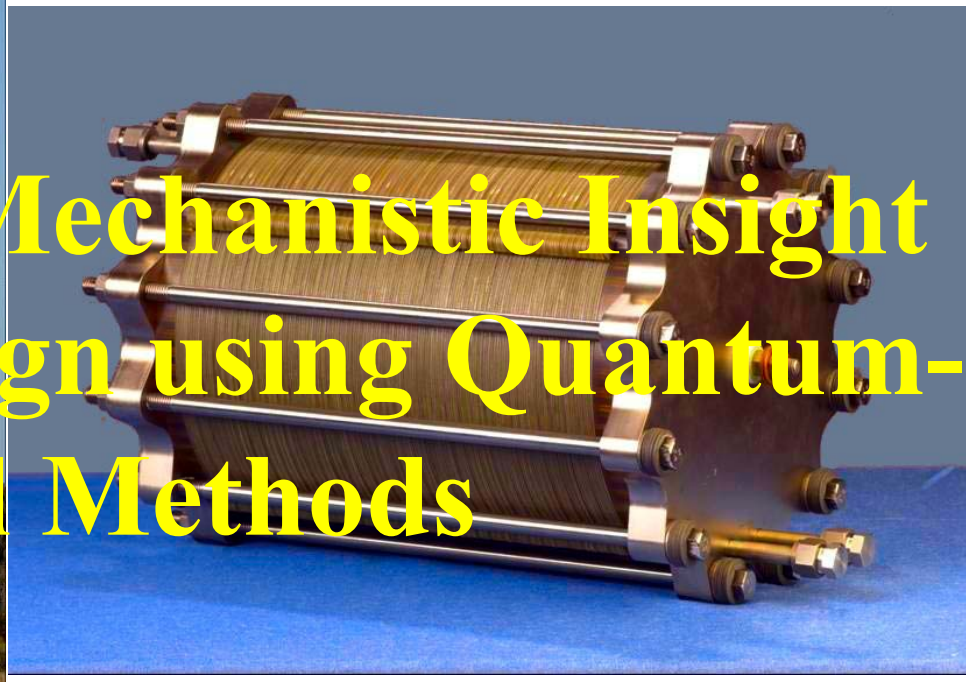
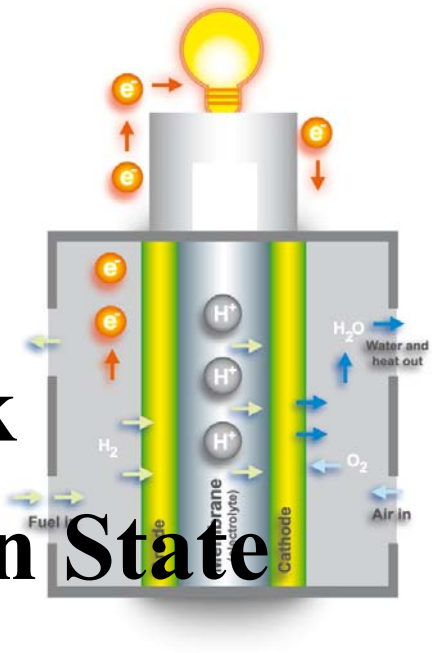




Electrocatalysis: Mechanistic Insight and Electrode Design using Quantum-Chemical Methods

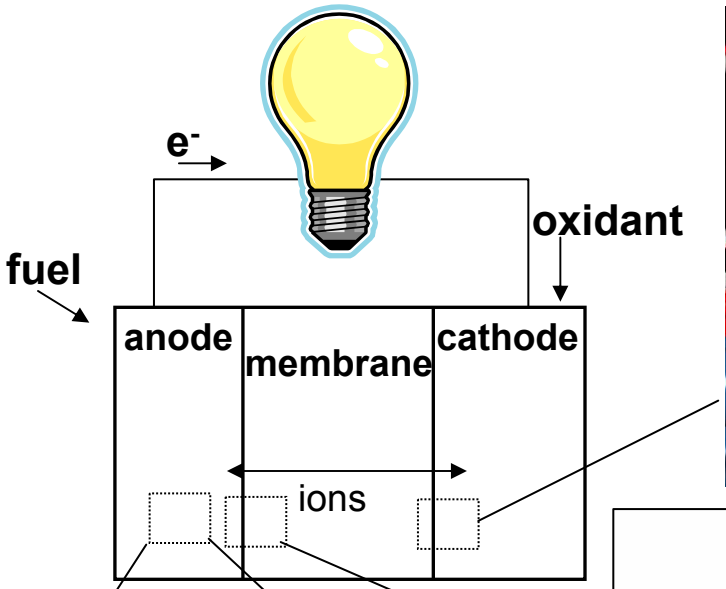


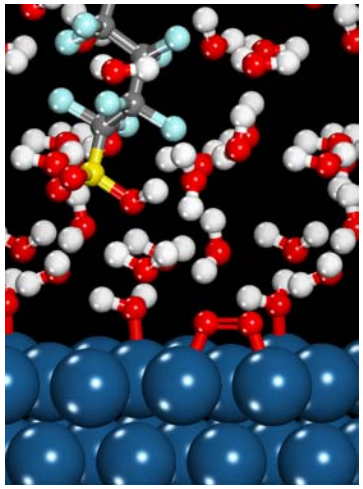
Michael J. Janik

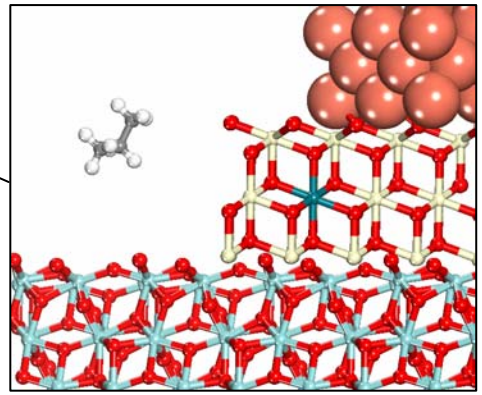
mjanik@psu.edu, Penn State

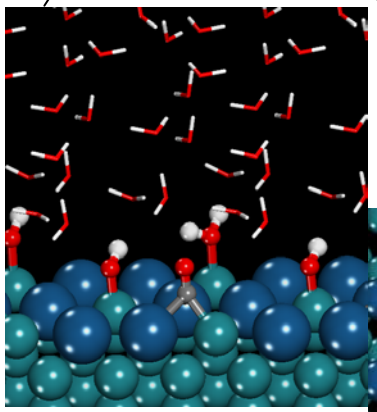
Computational Design of Electrode Materials for Fuel Cells

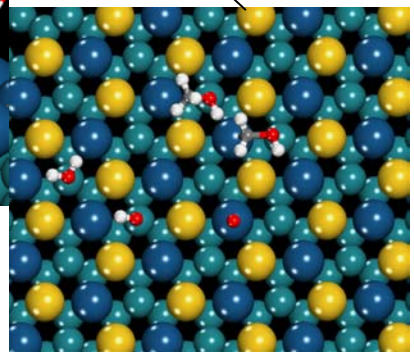
Mike Janik Research Group, Chemical Engineering mjanik@psu.edu











•**Aqueous Environments**

•**Complex interfaces**

•**Alloy Design**

Methods:

Computational algorithms based on quantum mechanics

Novel approaches to including electrode potential variation

Applications:

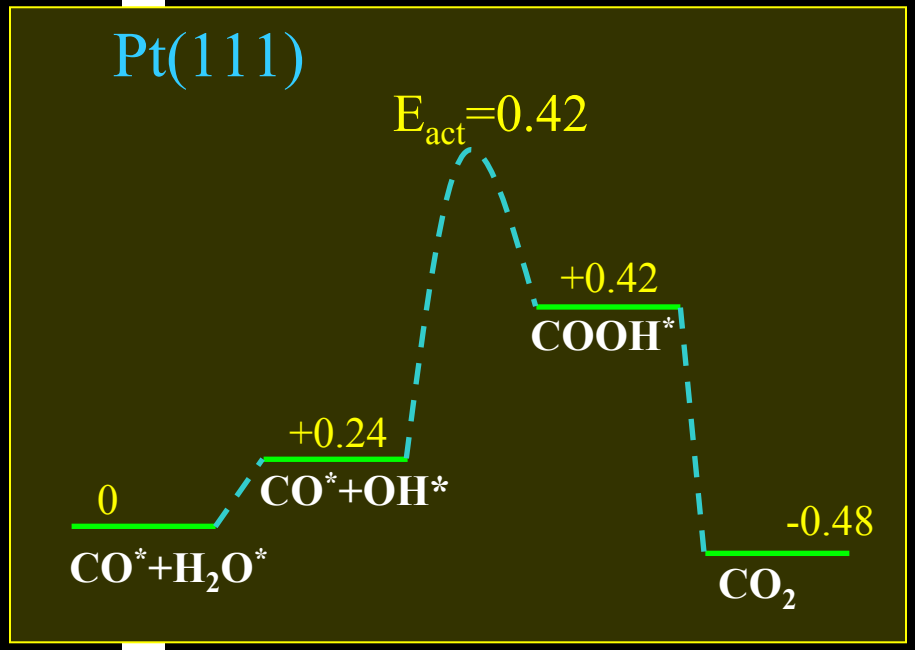
Alternative fuels & platforms:
- Borohydrides & Alkaline Cells
- Hydrocarbons & Solid Oxide Cells

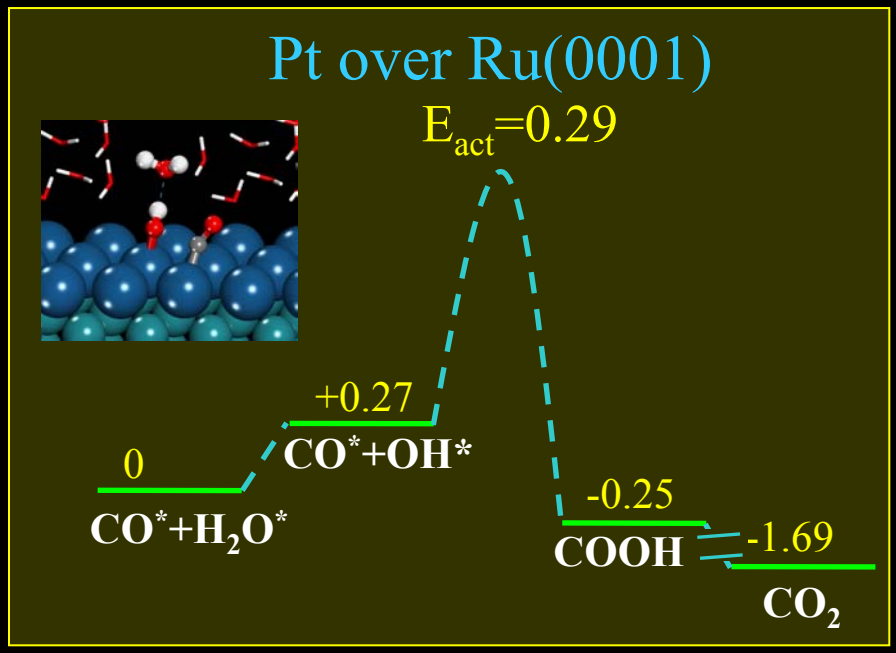
Improved efficiency and power:
- Oxygen Reduction at the Electrode-Membrane Interface
- Poisoning and Promotion Mechanisms

Quantum-Chemical Methods

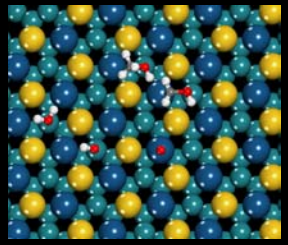
Schrödinger's equation $H\Psi=E\Psi$

Explain at an atomic level what controls catalyst performance

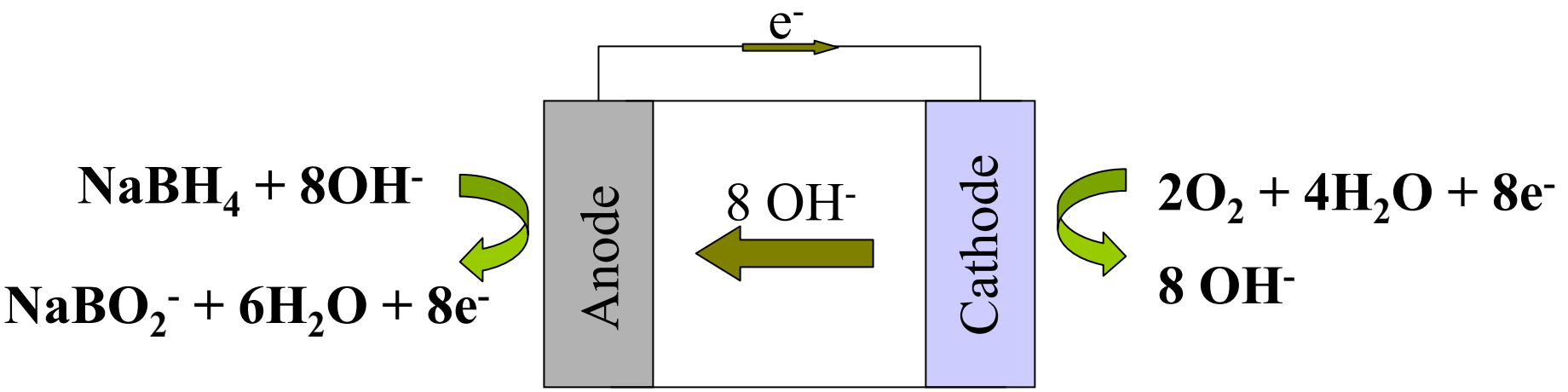




Virtual lab: "computational experiments" to design new catalytic materials



Computational Design of Novel Low and Intermediate Temperature Fuel Cell Electrocatalysts



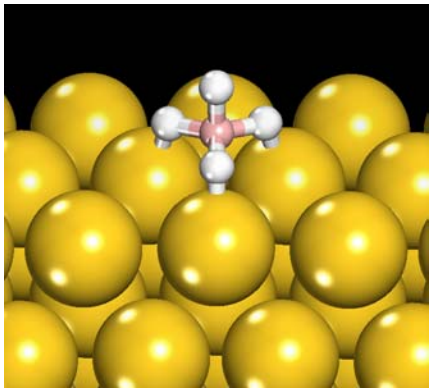
ΔG = -13 eV (1270 kJ/mol)

Applications - portable power (laptops, cell phones, automobiles(?), surge energy storage)

Project objectives:

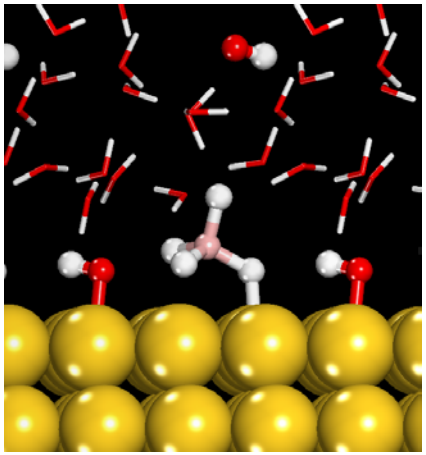
Determine reaction mechanisms and optimize the composition of electrocatalysts for novel fuel cell development

Computational Approach



gas phase model
reaction intermediates
binding sites
preliminary mechanism

add sequentially
coadsorption and kinetics
solvation
electric field



pure metal catalytic behavior
explain experimental observations

test catalyst design
improvements at the level
of complexity necessary