NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

Catalysts: The Philosopher’s Stones which will Orchestrate a Hydrogen Economy

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How is Hydrogen Produced Today ?

Fossil fuels like Methane/Coal

$CH_4 + H_2O \leftrightarrow CO + 3H_2, \Delta H = 206$ kJ/mol

Energy Intensive!
Pressure: 3-25 bar
Temperature: 700-1000°C

CO_2 footprint: ~ 10 tons of CO_2/ton of H_2
Cost: ~ 2.5 S$/kg
similar cost per energy compared to petrol

95%

Steam Methane Reformer, Praxair

Electrolyze Water

$2H_2O \leftrightarrow 2H_2 + O_2, \Delta H = 285$ kJ/mol

Electric potential: ~ 1.7 V
Pressure: 1 bar
Temperature: 25°C

CO_2 footprint: ~ 2-3 tons of CO_2/ton of H_2
Cost: ~ 6.4 S$/kg
3x higher cost per energy compared to petrol

5%

Water electrolyser, McPhy Energy

Hydrogen as a Storage for Excess Renewable Electricity

PNAS

CrossMark
click for updates

Round-the-clock power supply and a sustainable economy via synergistic integration of solar thermal power and hydrogen processes

Emre Gençer[a], Dharik S. Mallapragada[a], François Maréchal[b], Mohit Tawarmalani[c], and Rakesh Agrawal[a,1]

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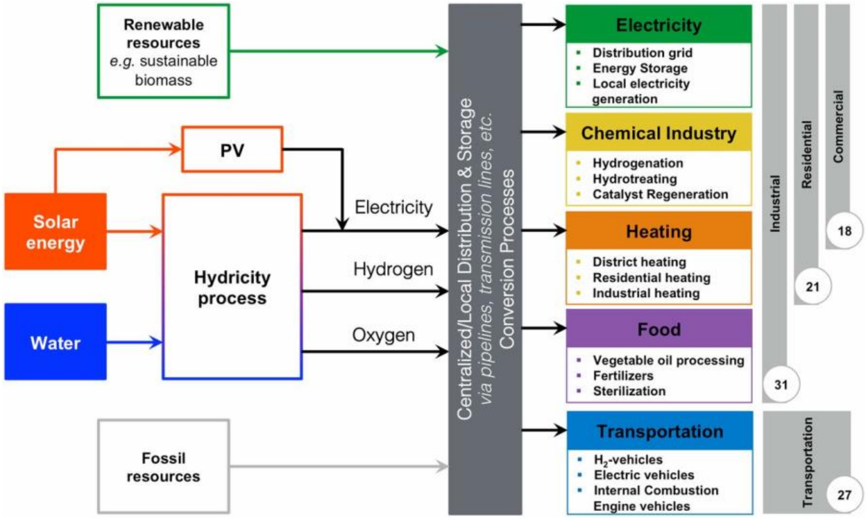
Hydridicity: Synergistic production of electricity and H_2 in in a solar thermal power plant

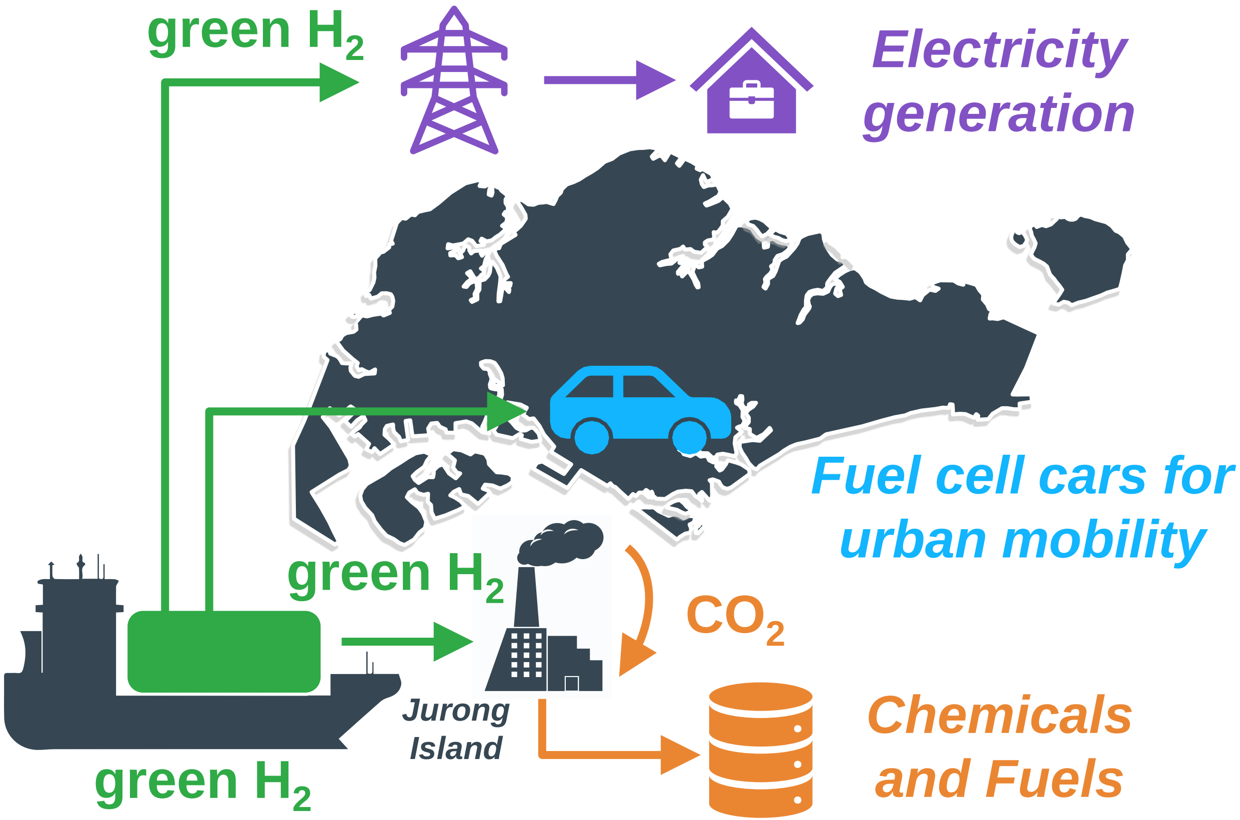
Produce H_2 from sunlight when daily electricity demand drops. Use stored H_2 for electricity generation at night/cloudy days. H_2 can be integrated with chemical production too.

Hydridicity process integrated with electricity and chemicals production



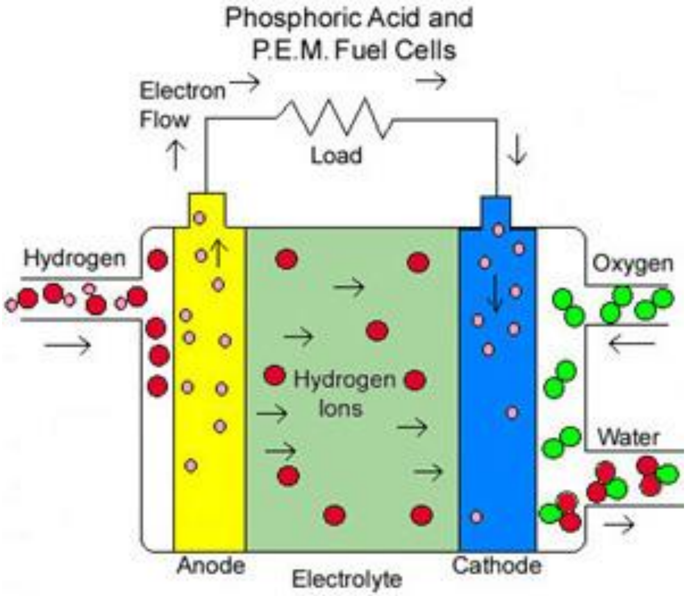
Gencer et al. **PNAS,** 112, (2015), 15821

The role of Hydrogen in Singapore's Energy Roadmap



Fuel Cells

Fuel cells combust H_2 & O_2 generating energy with H_2O as the only by product



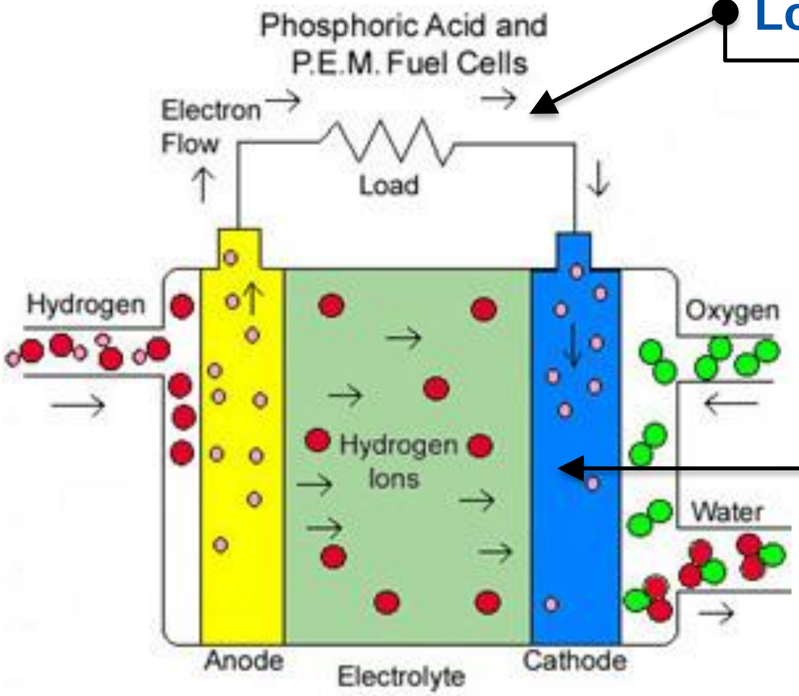
Smithsonian Institute

Vehicles
Toyota Mirai

Aircraft
Airbus (planned)

Cruise Ships
Norway
(planned)

Hurdles Limiting the Widespread Use of Fuel Cells



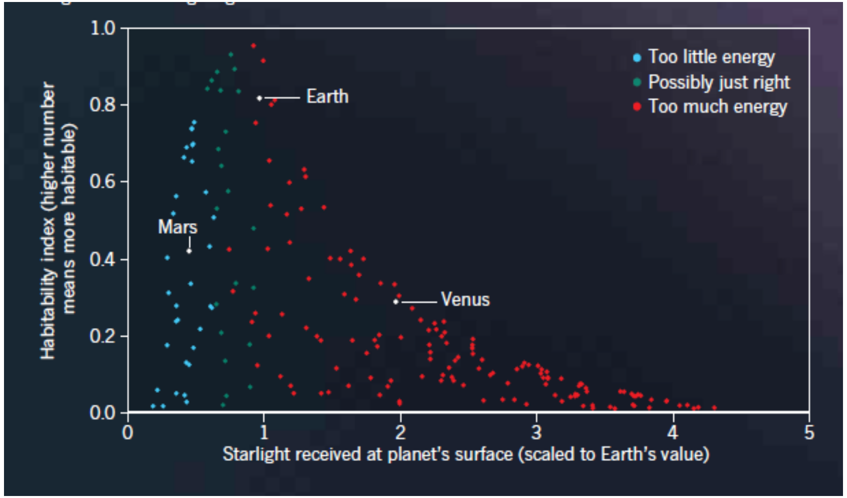
Smithsonian Institute

Load: Motor in a vehicle

Cathode: O_2 reduced to H_2O

- Sluggish reaction rate
- Requires a Pt catalysts
- **Fuel cell car: 60 g of Pt**
- Catalytic converters in gasoline-powered cars: 6 g of Pt
- **Need Pt replacements with similar performance and durability, but half the cost.**

The Goldilocks Principle: From Catalyst Design to Discovering Alien Life



A. Witze **Nature,** 527, (2015), 288

The Goldilocks principle

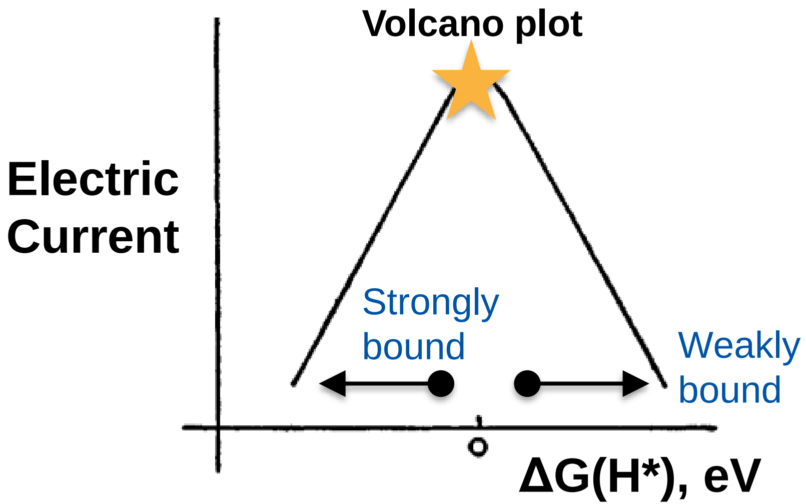
It is a scientific concept stating that something must fall within margins as opposed to reaching extremes.

- **Planets which can sustain life must be neither too hot nor too cold.**
- The starlight received by a planet is related to the habitability index (likelihood of liquid water).

The Goldilocks Principle in Catalysis

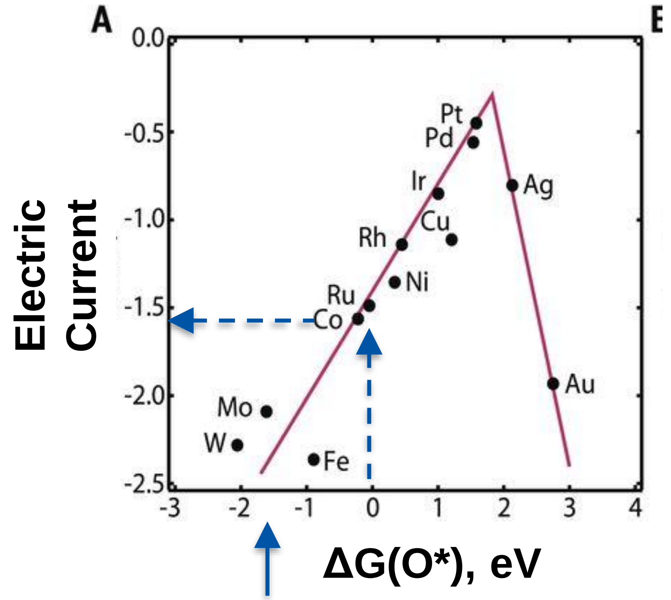
Sabatier Principle: Bests catalysts bind molecules neither too strongly nor too weakly.

Hydrogen evolution reaction in water splitting



R. Parsons, **Trans. Faraday Soc.** 54, (1958), 1053.

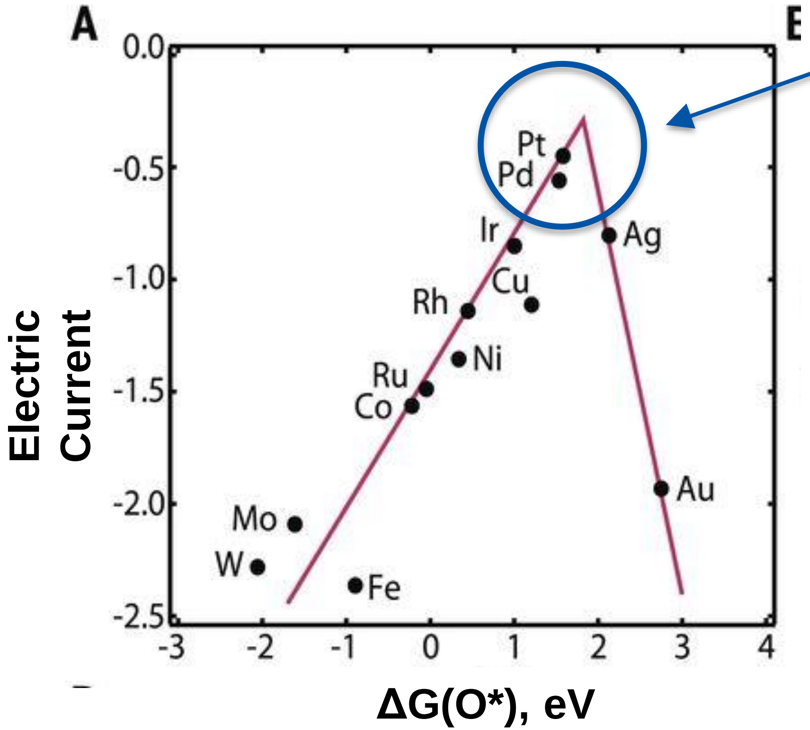
Oxygen reduction reaction in fuel cells



Calculate the binding strength of molecules using Quantum Mechanics

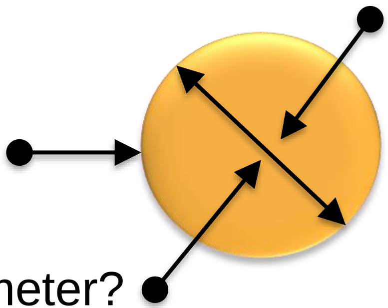
J. Norskøv et al., **J. Phys. Chem. B.** 108, (2004), 17886.

Challenges with Existing Volcano Plots for Oxygen Reduction



J. Norskøv, et al. **J. Phys. Chem. B.** 108, (2004), 17886.

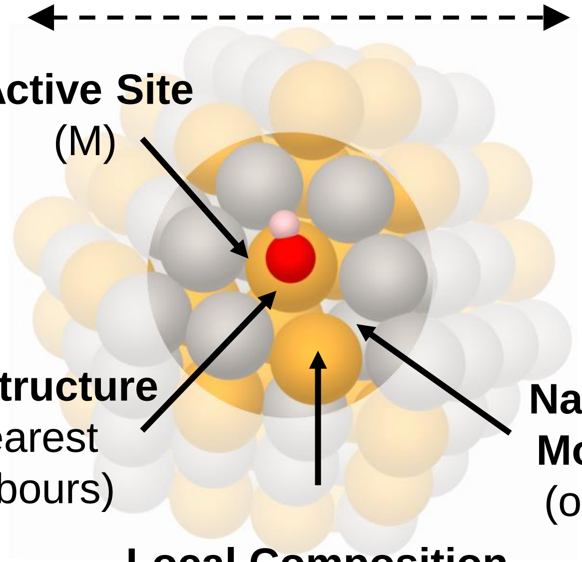
Pt-based materials are the best catalysts for oxygen reduction in fuel cells



Volcano plots cannot prescribe specific nanoparticle – morphologies, – diameter, & – compositions. These inputs needed for experimental synthesis.

Designing Catalysts using Atoms as "Lego Blocks"

Deconstructing a Nanoparticle

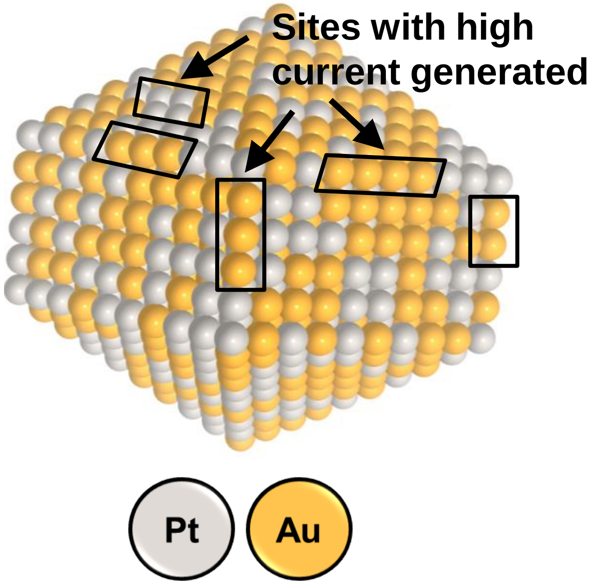


- **Size:** How many Atoms?
- **Shape:** How are atoms arranged?
- **Composition:** What is the ratio of M:N in the nanoparticle?

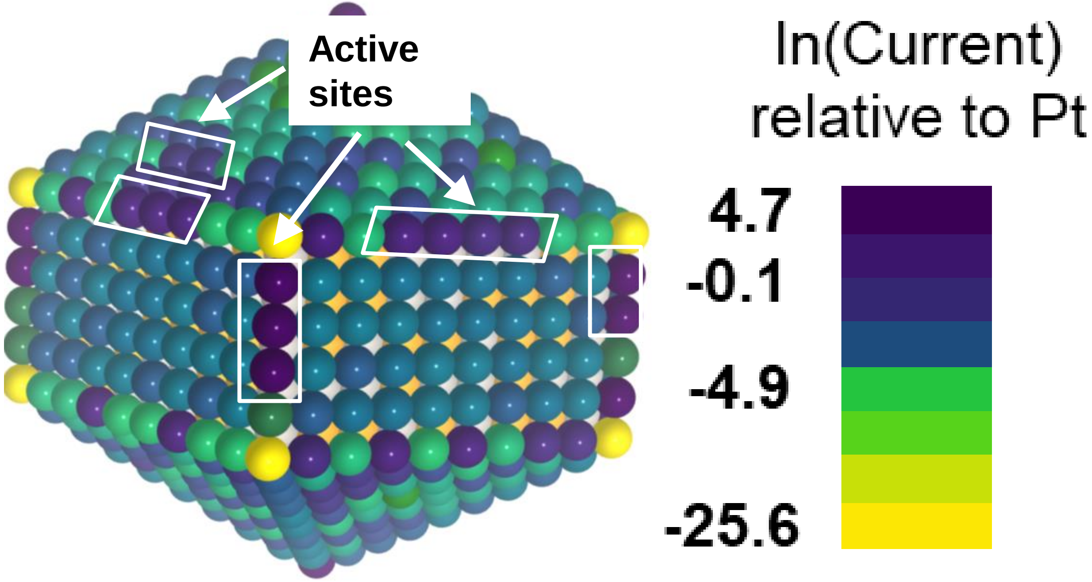
Can we deploy quantum mechanics and machine learning to evaluate active-site-specific reaction rates for a nanoparticle having any size, shape, and composition?

Estimating Electrical Current in Fuel Cells with Atomic Level Precision

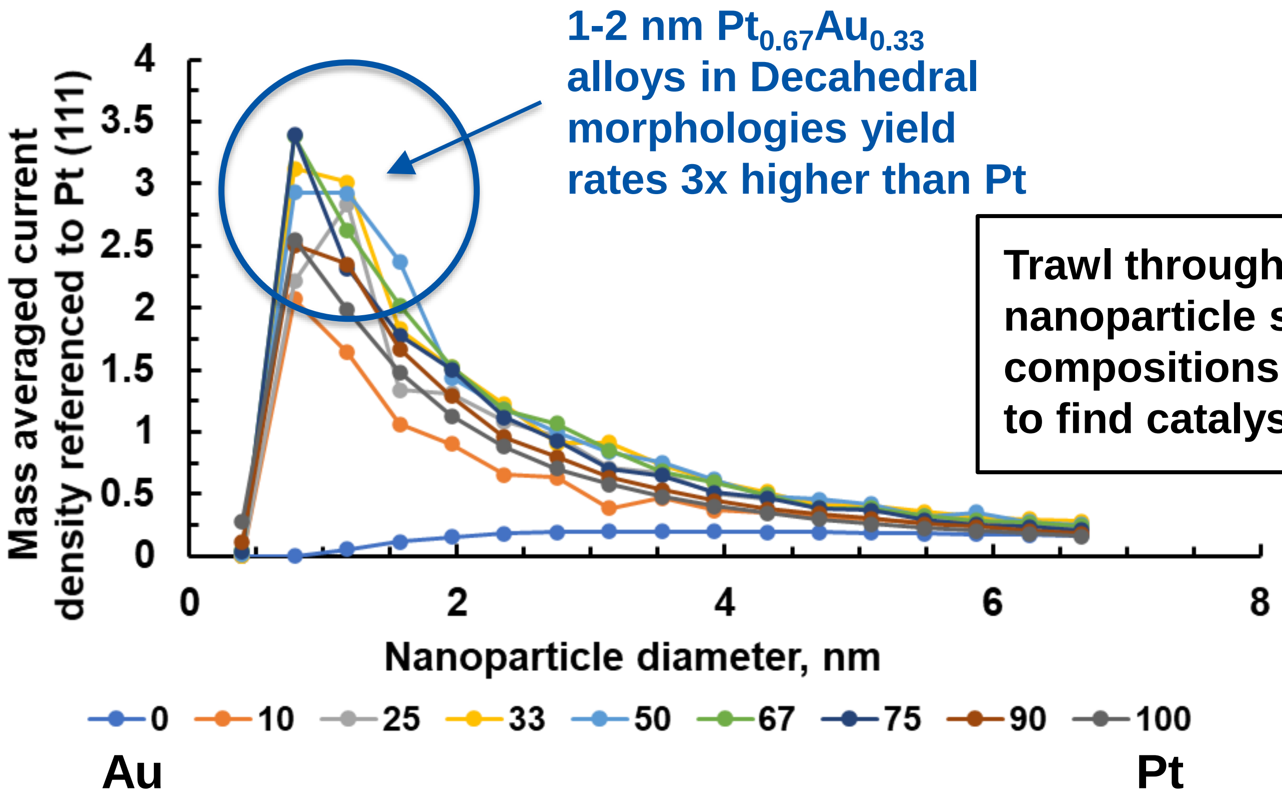
(a) $Pt_{982}Au_{983}$ decahedron



(b) Active site specific current density



Designing Catalysts using Atoms as “Lego blocks”

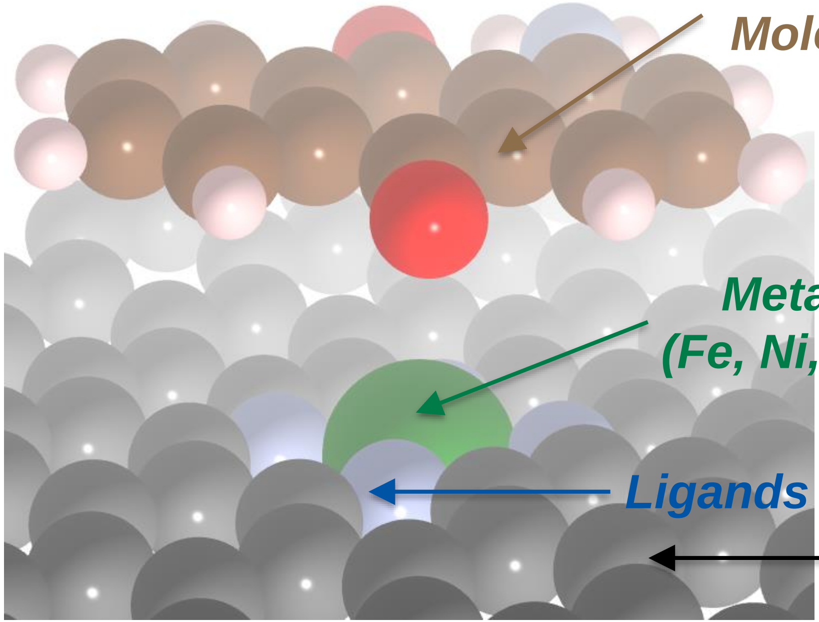


Trawl through a wide-range of nanoparticle sizes, shapes, and compositions using our framework to find catalysts better than Pt

Beyond Pt: Enzyme-Inspired Earth-Abundant Catalysts for Fuel Cells

Prof. Wang Xin
Chair, School of Chemical and Biomedical Engineering, NTU

Dr. Xiaogang Li

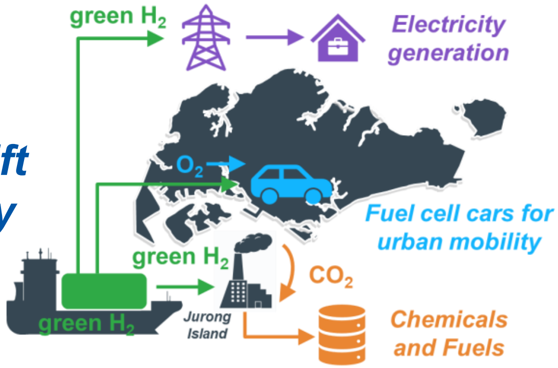


X. Li et al., **Adv. Mater.** (2021), 2104891.

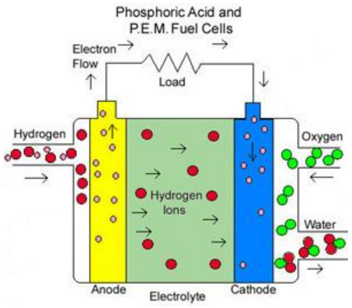
Together with experimental collaborators, tailor the earth-abundant metal site, ligands, and molecular confinement to find catalysts better than Pt

Takeaway Messages

Singapore's shift to a H_2 Economy



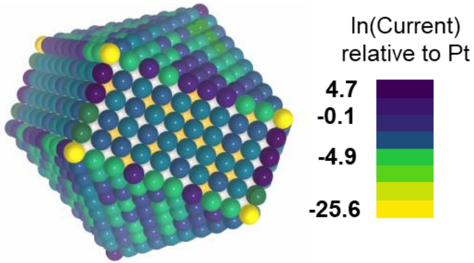
Fuel Cells for Transportation



Requires Pt catalysts

Need to find replacements with similar performance and durability, but 2x cheaper

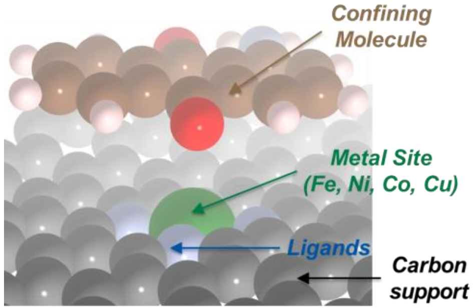
Computational Design of Fuel Cell Catalysts



Determine atom-specific performance of fuel cells

Accelerate search for nanoparticles beyond Pt

Enzyme Inspired Earth Abundant Catalysts



Tailor metal sites, ligands, and confining molecules to maximize current generated