Fuel Cells and a Nanoscale Approach to Materials Design

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Outline

PEM fuel cells (issues)

A nanoscale approach to materials design

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What is a fuel cell?

A fuel cell is an electrochemical device that combines hydrogen and oxygen to produce electricity, with water and heat as its by-product.

As long as fuel is supplied, the fuel cell will continue to generate power.

Since the conversion of the fuel to energy takes place via an electrochemical process, not combustion, the process is clean, quiet and highly efficient – two to three times more efficient than fuel burning.

Benefits

•low or zero emissions,

•high efficiency and reliability,

•multi-fuel capability

•siting flexibility, durability, scalability

•ease of maintenance.

•fuel cells operate silently, so they reduce noise pollution as well as air pollution

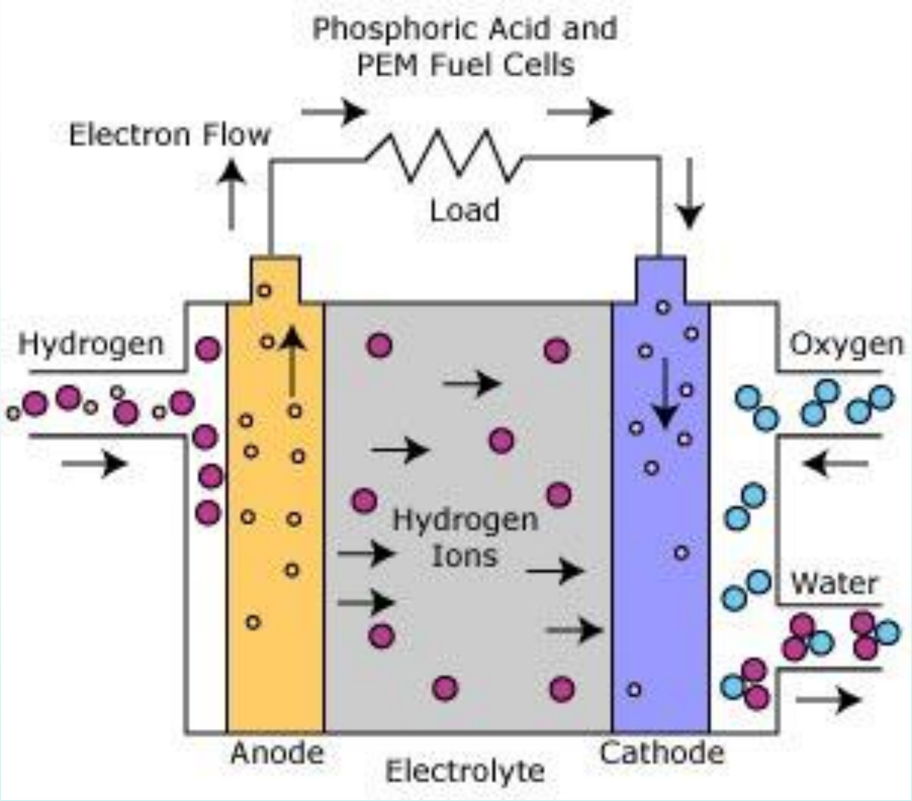
•waste heat from a fuel cell can be used to provide hot water or space heating for a home or office.

PEM Fuel Cell Technology

Proton Exchange Membrane
or
Polymer Electrolyte Membrane

- Membrane is a permeable polymer sheet which allows protons (H atoms) to pass through
- Operate at low temperatures with high power density
- Low cost, small size, high performance
- Ideal for transportation, stationary and portable applications

Energy Storage and Conversion: Fuel Cells



Efficiency issues:

Membrane transport

Anode:
Impurity-tolerant catalyst

Cathode:
A good catalyst for oxygen reduction reaction (ORR) ($1/2O_2+2H^++2e^- = H_2O$)

Catalyst Issues

(1) Substantial overpotential for the ORR reduces the thermal efficiency to 43% at 0.7 V [compared to 87% at reversible ORR potential (1.23 V)]

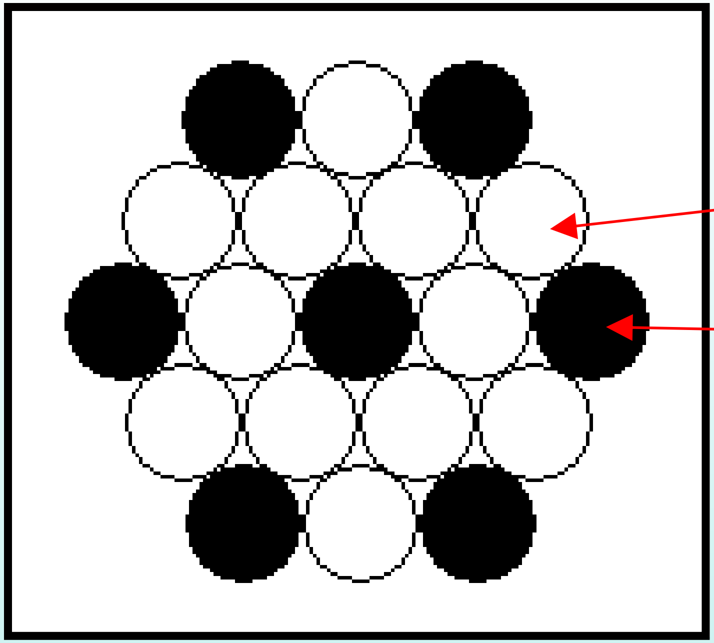
(2) Pt is expensive (Pt-loading)

(3) Performance degrades too quickly due to dissolution (stability issue)

Question: Can we use modern experimental methods to design a nanoscale catalyst?

Tailoring surface properties at the atomic level

Bimetallic Pt-alloy surfaces - Pt_3M



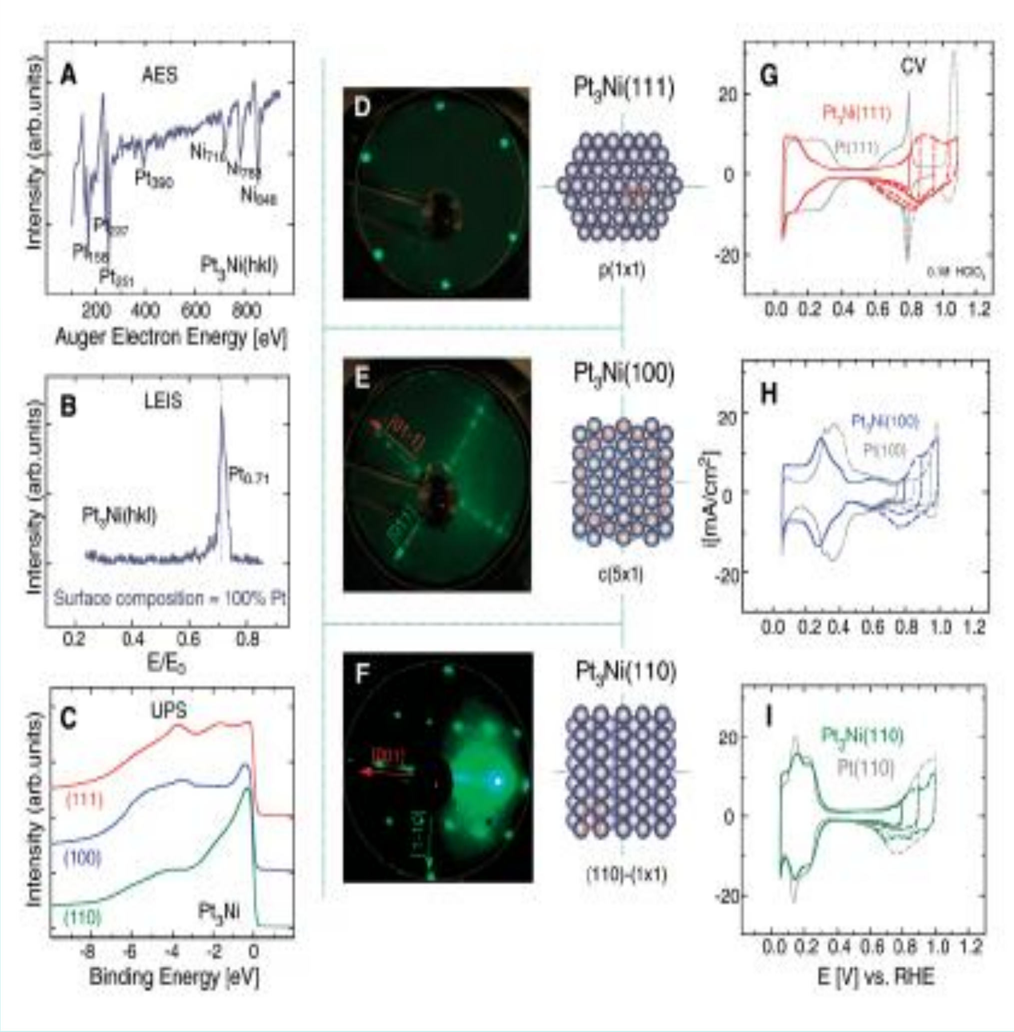
Bifunctional effects:

Pt for catalysis

M to do something else?

Effects can be: (1) Ensemble (2) Electronic

Model Electrocatalysts: Pt_3Ni crystals

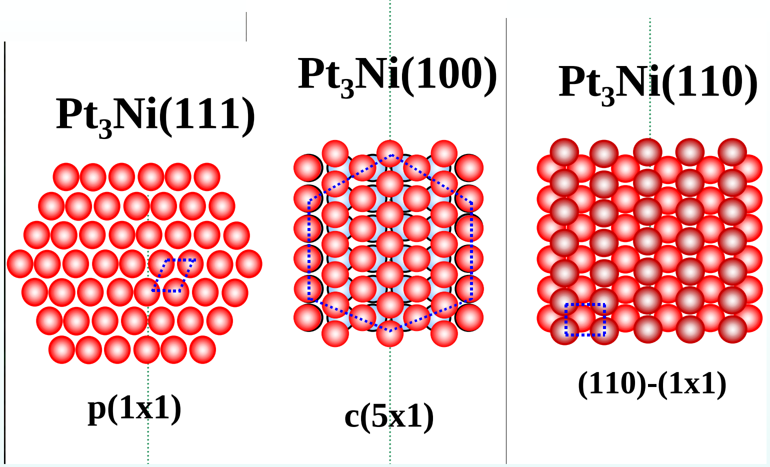


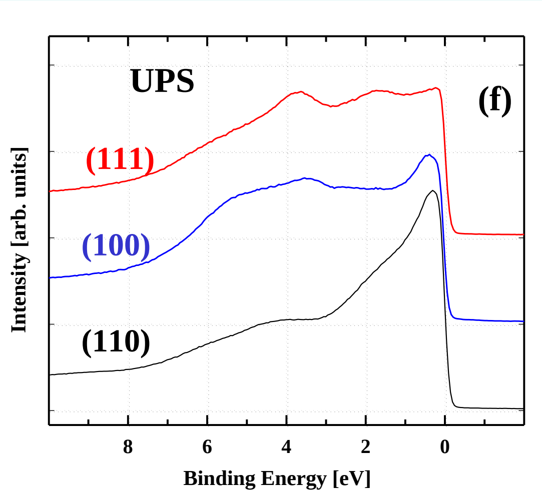
Key results from combined studies:

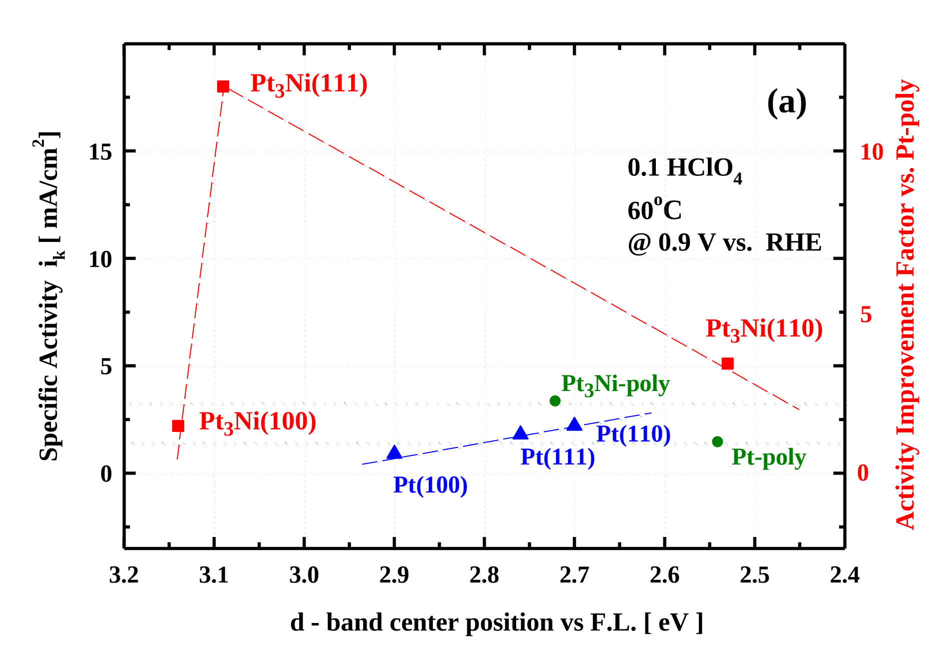
(1) Surfaces are 100% Pt

(2) Segregated surfaces are stable during reactions

(3) Activity depends on atomic geometry







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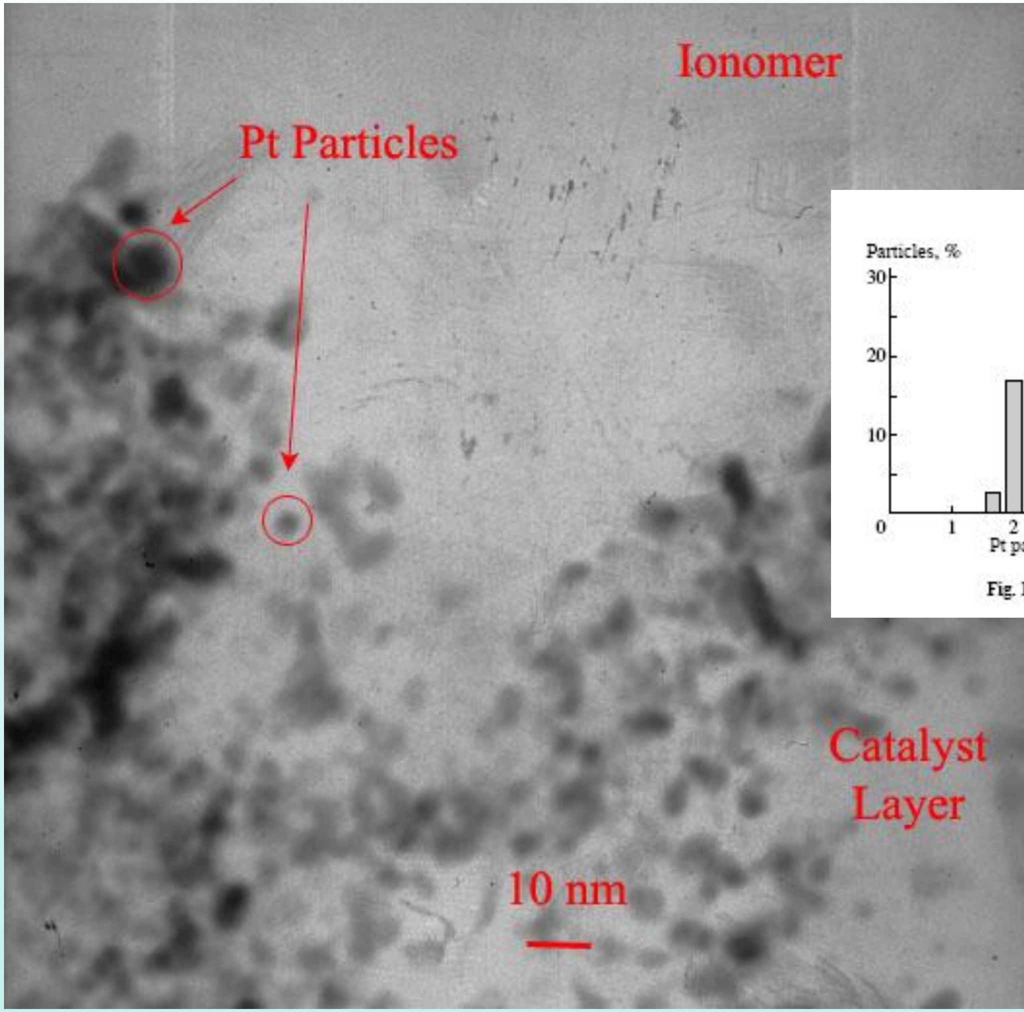
<u>Real</u> catalysts are nanoparticle arrays



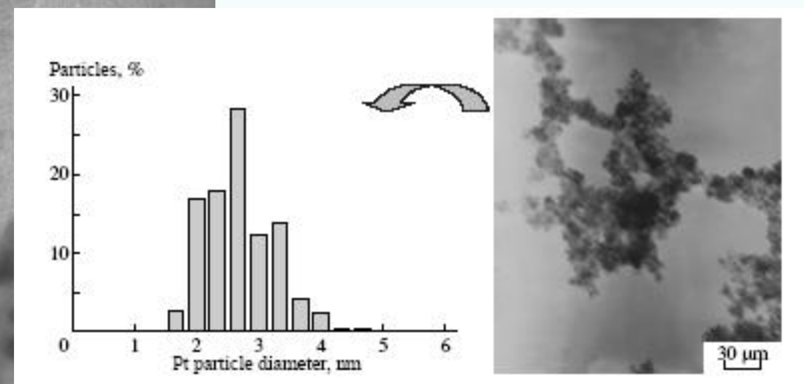
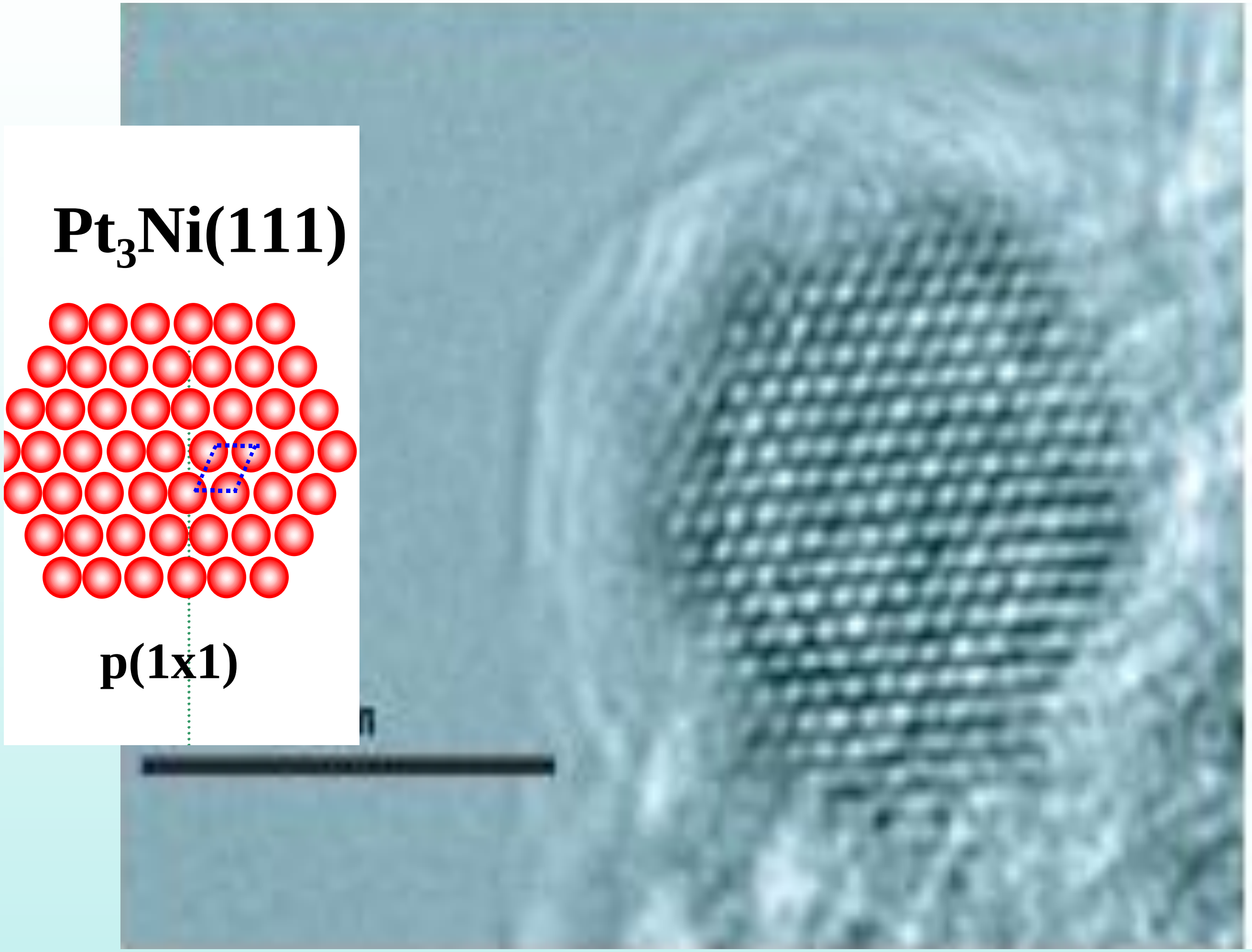
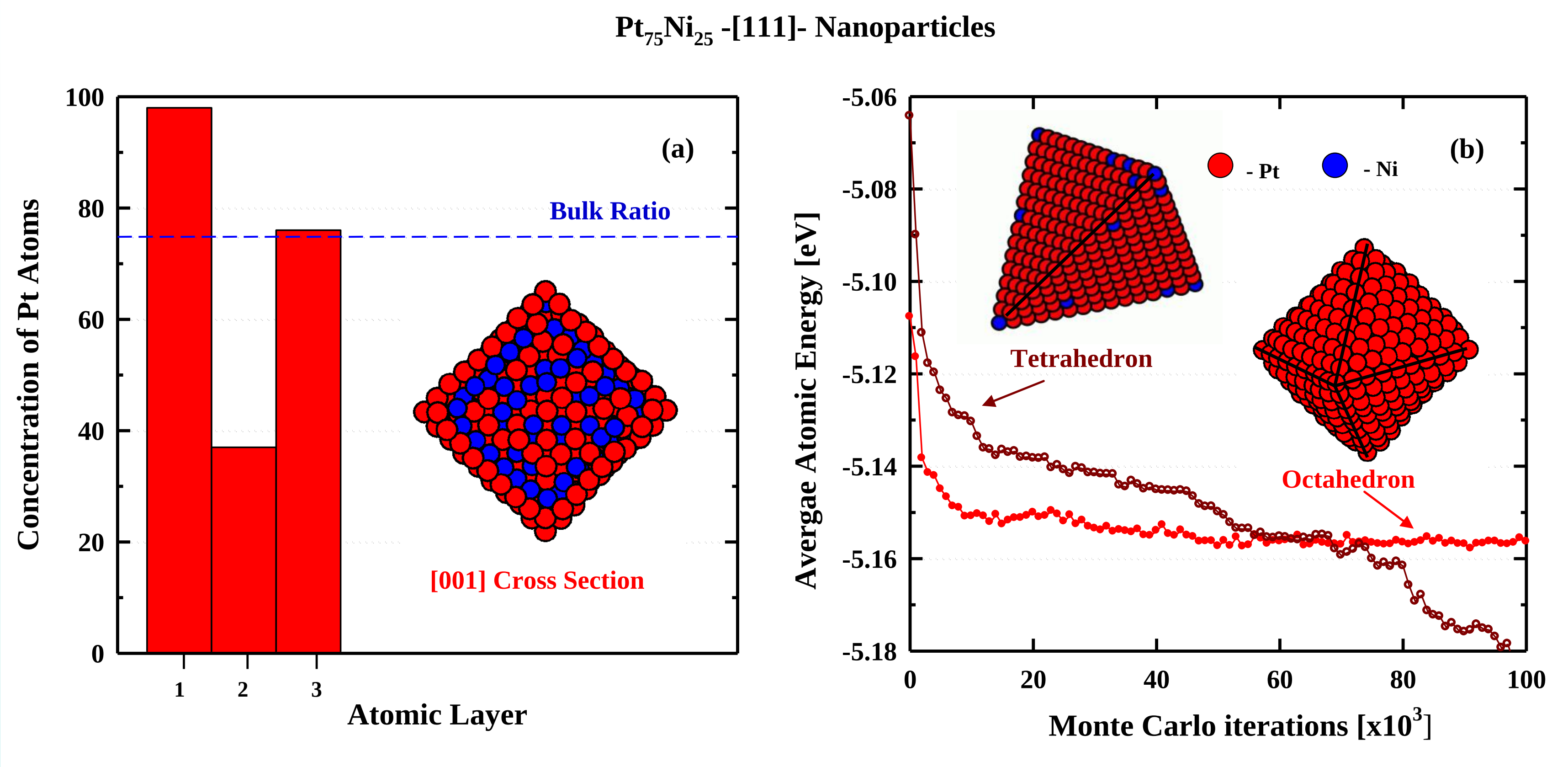


Fig. 10. TEM micrograph and particle size distribution of Pt catalyst.

TEM shows nanoparticles governed by ECS



DFT and Monte-Carlo calculations for nanoparticles



These nanoparticles have yet to be engineered

Summary

- Fuel cells offer significant potential climate and energy security benefits

- Materials design from fundamental nanoscale studies

- This approach could be used in a range of materials (and energy) applications