

# HIGHLY DISPERSED ALLOY CATHODE CATALYST FOR DURABILITY

---

T. D. Jarvi  
UTC Power Corporation  
17 May 2007



**UTC Power**

A United Technologies Company

Project ID # FCP 26

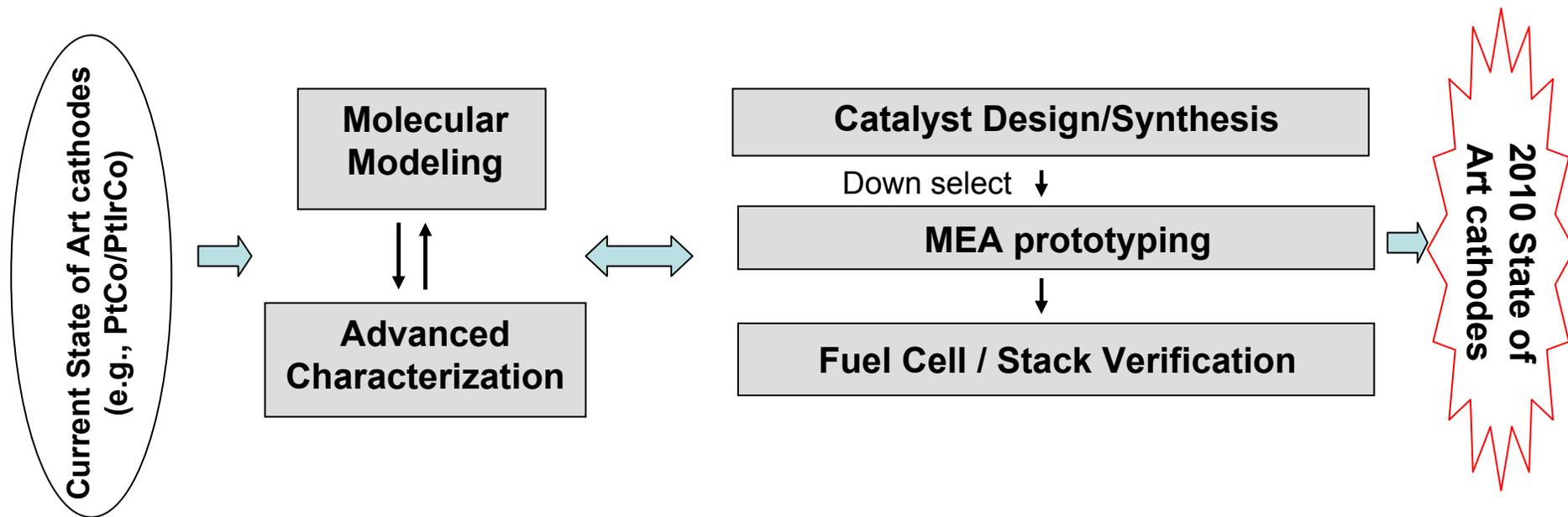
# HIGHLY DISPERSED ALLOY CATALYST

## Objectives of project

Characteristic	DOE 2010 Target
Pt group metal Total Content	0.50 g/kW rated
Pt group metal Total Loading	0.30 mg PGM/cm <sup>2</sup>
Durability with cycling $\leq 80^{\circ}\text{C}$ ; $> 80^{\circ}\text{C}$	5000 h; 2000 h
Electrochemical Area Loss	< 40 %
Mass Activity at 900 mV <sub>RHE</sub> (IR-Free)	0.44 A/mg Pt
Specific Activity at 900 mV <sub>RHE</sub> (IR-Free)	720 $\mu\text{A}/\text{cm}^2$
Cost	\$8/kW

# HIGHLY DISPERSED ALLOY CATALYST

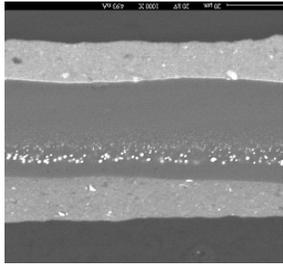
## Program approach



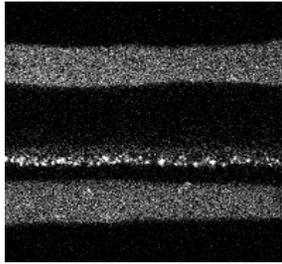
# HIGHLY DISPERSED ALLOY CATALYST

---

## Understanding high performance materials

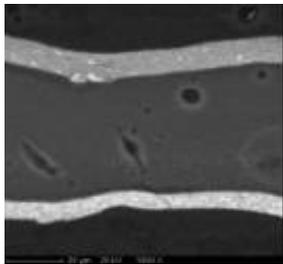


B.S.E.

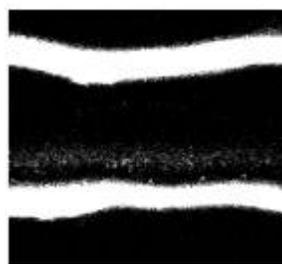


Pt

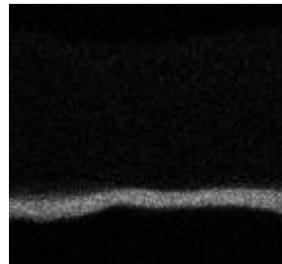
**Pt/C cathode**



B.S.E.

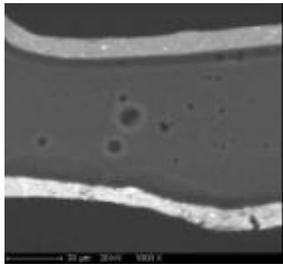


Pt

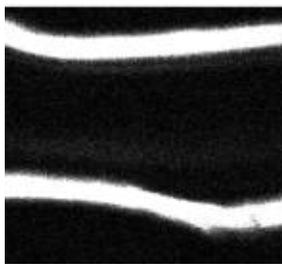


Co

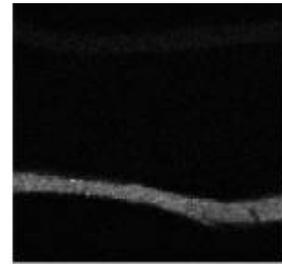
**PtCo/C cathode**



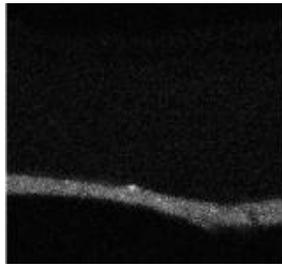
B.S.E.



Pt



Co

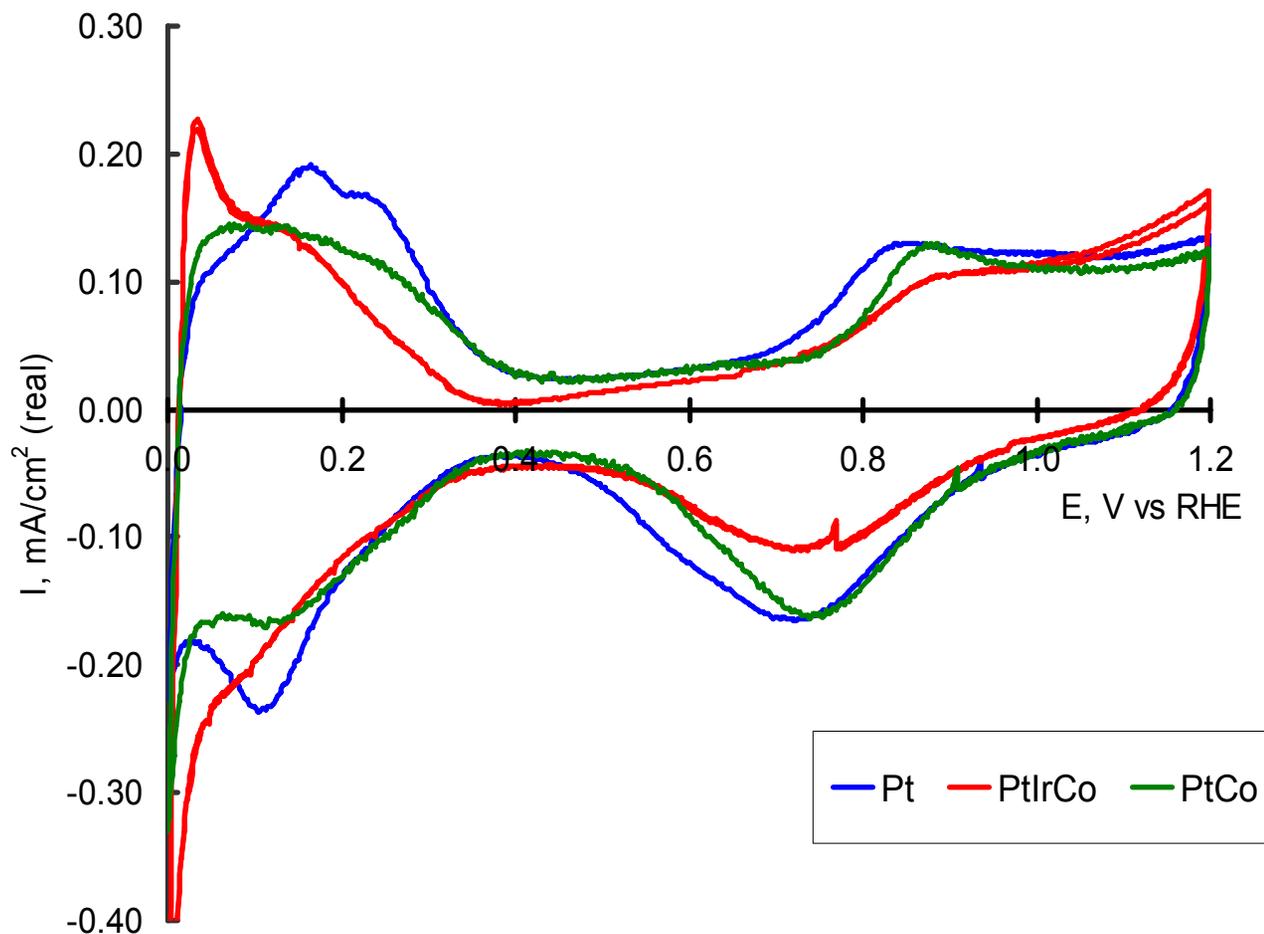


Ir

**PtIrCo/C cathode**

# HIGHLY DISPERSED ALLOY CATALYST

## Understanding high performance materials

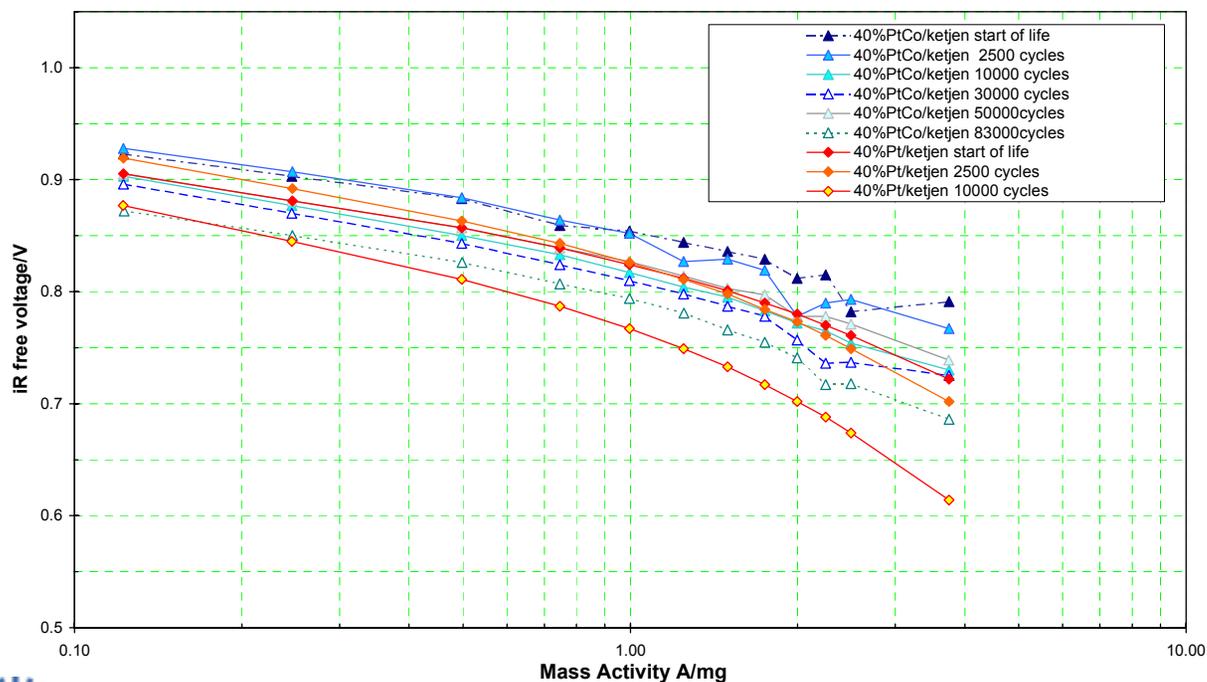


# HIGHLY DISPERSED ALLOY CATALYST

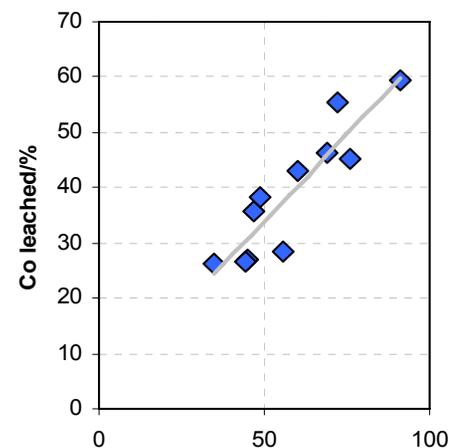
## Understanding high performance materials

Pt alloy catalysts show higher mass activity than Pt (0.25-0.3A/mgPt for Pt alloy)  
 Pt alloy performance benefit retained after MEA voltage cycles 0.7-0.9V (iR-free)  
 Co is leached from PtCo alloys – decreases activity  
 Understanding these initial alloys drives future development

Cell at 80°C, Pressure 50/50 kPag, hydrogen/oxygen, 2/10 stoich, SH-30 membrane, Humidifier temperature 80/80°C



0.5M H<sub>2</sub>SO<sub>4</sub>, 363K, 24 hrs



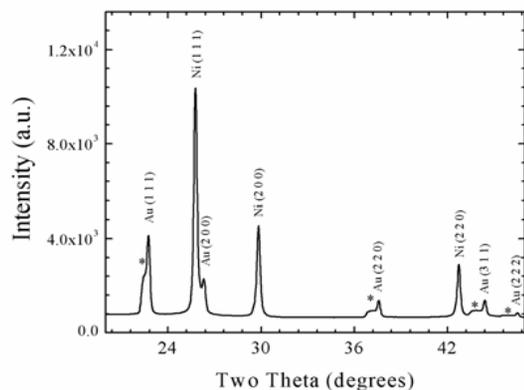
CO Chemisorption Metal Area/m<sup>2</sup>g<sup>-1</sup> Pt

Ex-situ acid leaching PtCo alloys shows Co removal strongly dependent on surface area/particle size

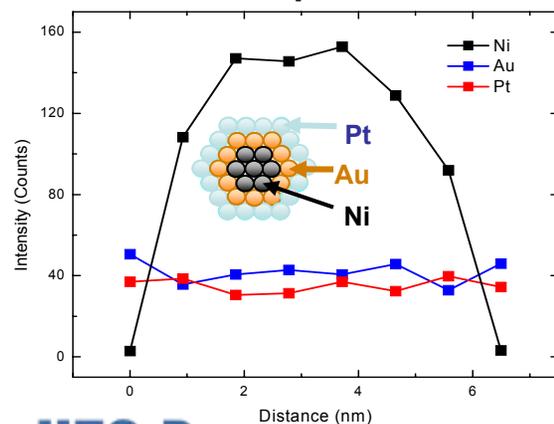
# HIGHLY DISPERSED ALLOY CATALYST

## Model systems to develop understanding

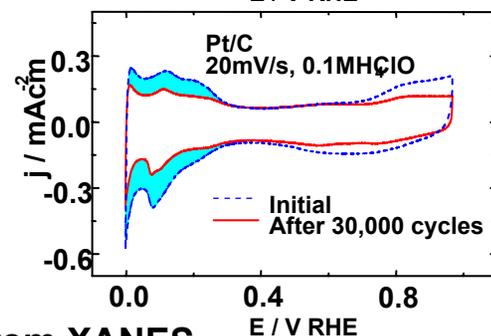
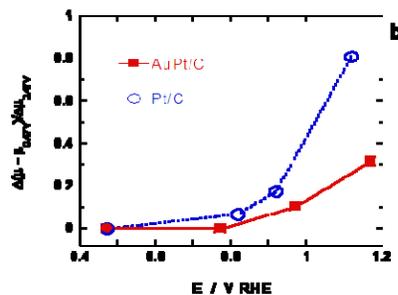
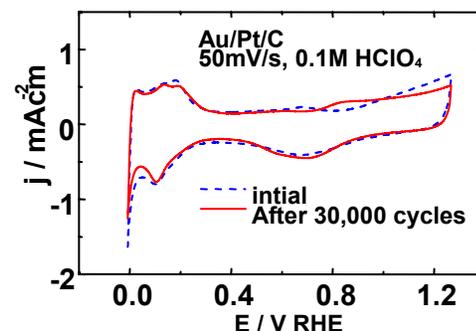
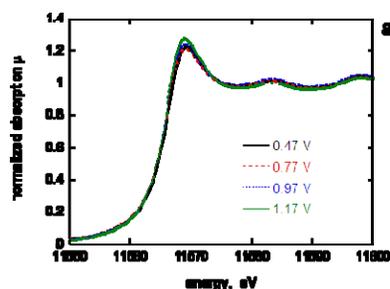
Segregation of Au in AuNi micro-powder x-ray diffraction



EDS of a Pt<sub>ML</sub>/Au/Ni nanoparticle in nano-probe mode



Learning from stabilization effects of Au clusters on Pt- no change in 30,000 cycles



Pt oxidation is decreased from XANES and Voltammetry

Au atoms may block the kink and step sites where PtO is formed first and Pt dissolution starts.



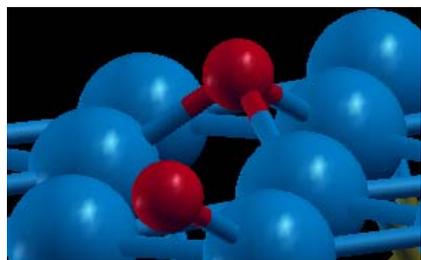
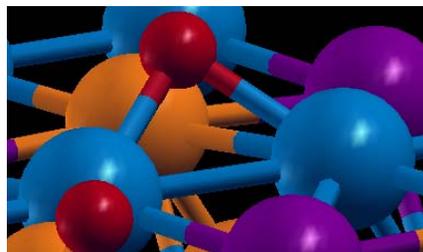
# HIGHLY DISPERSED ALLOY CATALYST

## Modeling to understand materials

### METHODS

Computational chemistry methods help to understand catalytic activity and metal dissolution

Thermodynamic analyses determine which alloys are more stable than Pt against dissolution



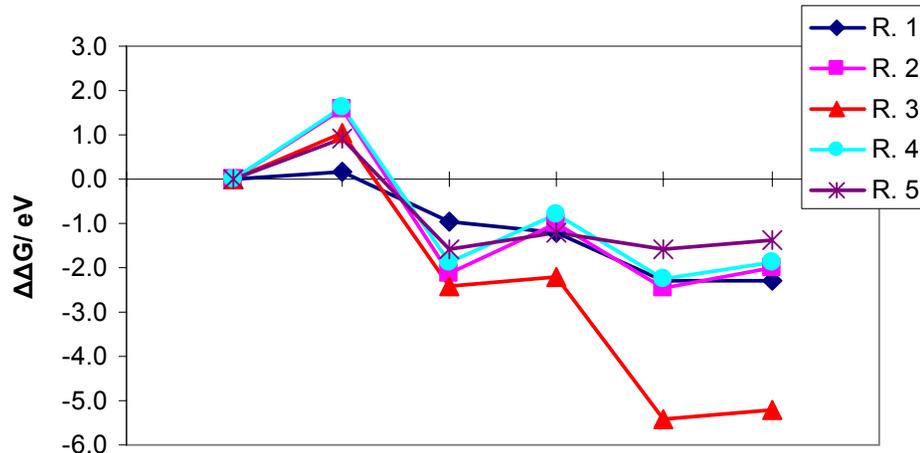
Oxygen attachment to atoms on the metal surface is the first step in the dissolution process

We calculate:

$$\Delta\Delta G_{rxni} = \Delta G_{rxni}|_{Alloy} - \Delta G_{rxni}|_{Pt}$$

If  $\Delta\Delta G < 0$  alloy atom easier to dissolve than Pt

If  $\Delta\Delta G > 0$  alloy atom more stable than Pt



Gu and Balbuena, JPCB 2006



TEXAS A&M UNIVERSITY  
DEPARTMENT OF CHEMICAL  
ENGINEERING

Perla B Balbuena  
balbuena@tamu.edu

# HIGHLY DISPERSED ALLOY CATALYST

---

## Program team



Catalyst fundamentals  
Catalyst development  
Verification



Catalyst development : alloys,  
supports, MEA Prototyping



Catalyst development : supports



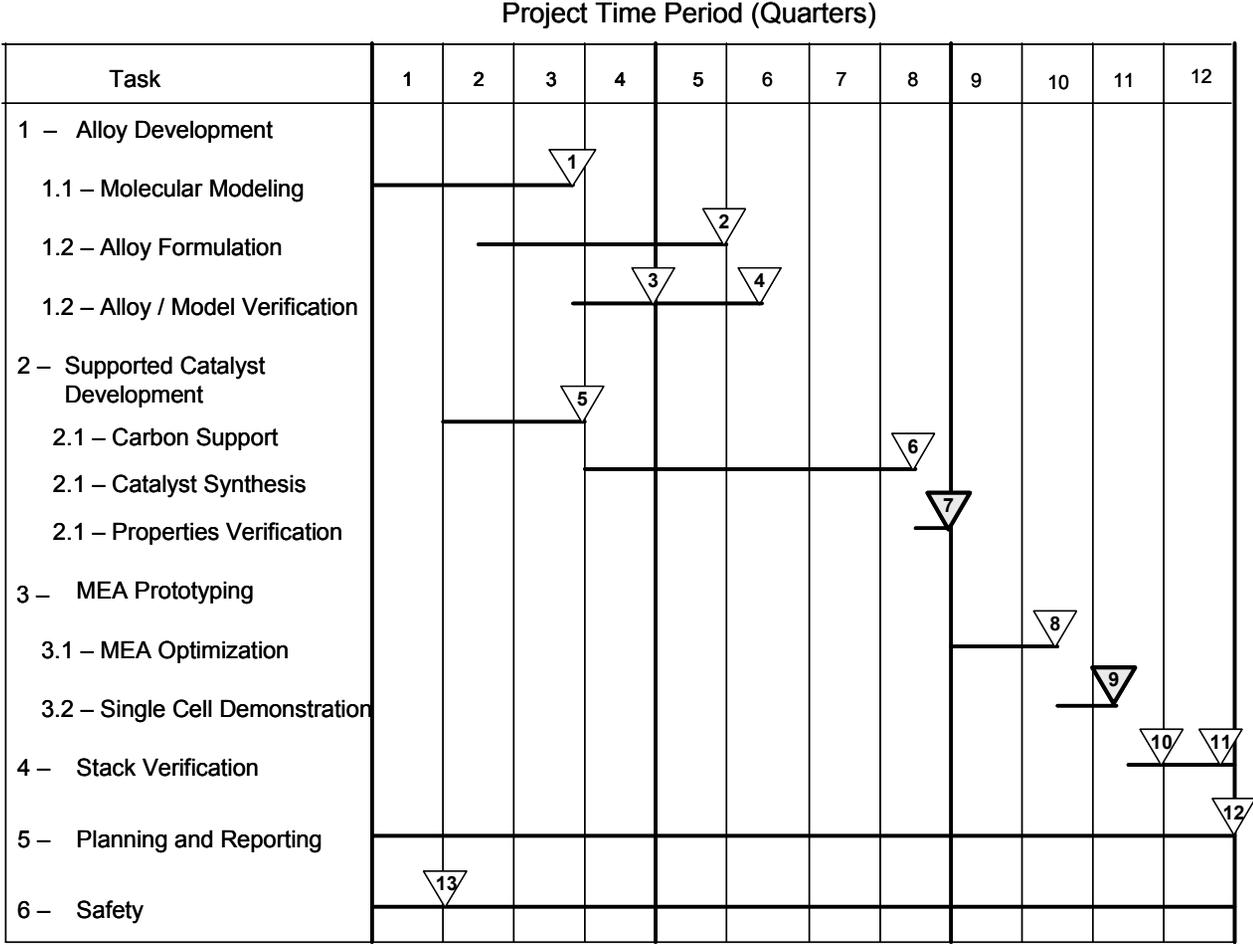
Catalyst fundamentals: experimental



Catalyst fundamentals: modeling

# HIGHLY DISPERSED ALLOY CATALYST

## Project timeline



Legend — Task    ▽ Milestone    ▽ Go/No-Go



**UTC Power**

A United Technologies Company

# HIGHLY DISPERSED ALLOY CATALYST

## Program budget (total program)

Government Fiscal Year '07	\$2,214,267
Government Fiscal Year '08	\$2,868,363
Government Fiscal Year '09	\$2,736,472
Government Fiscal Year '10	\$669,319

Cost share – 25%