### HIGHLY DISPERSED ALLOY CATHODE CATALYST FOR DURABILITY

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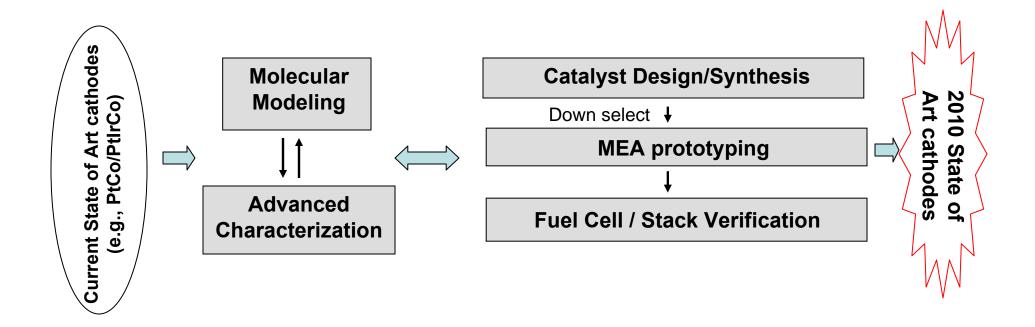
# HIGHLY DISPERSED ALLOY CATALYST Objectives of project

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



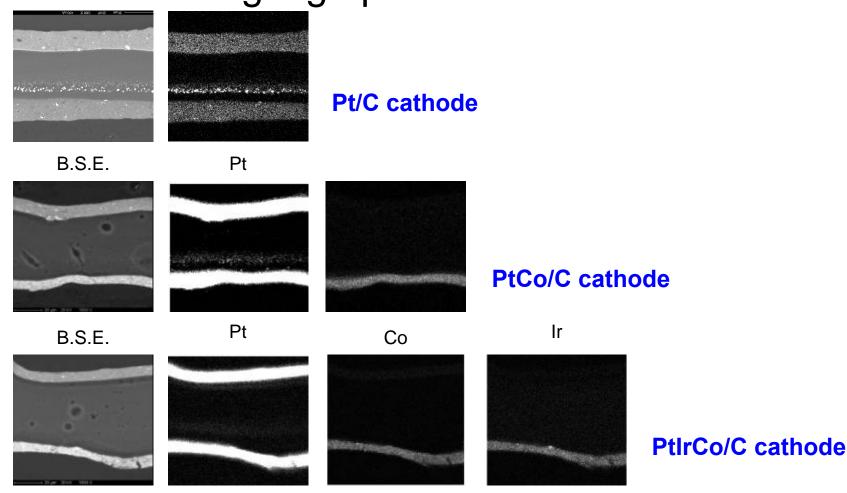
# HIGHLY DISPERSED ALLOY CATALYST

#### Program approach



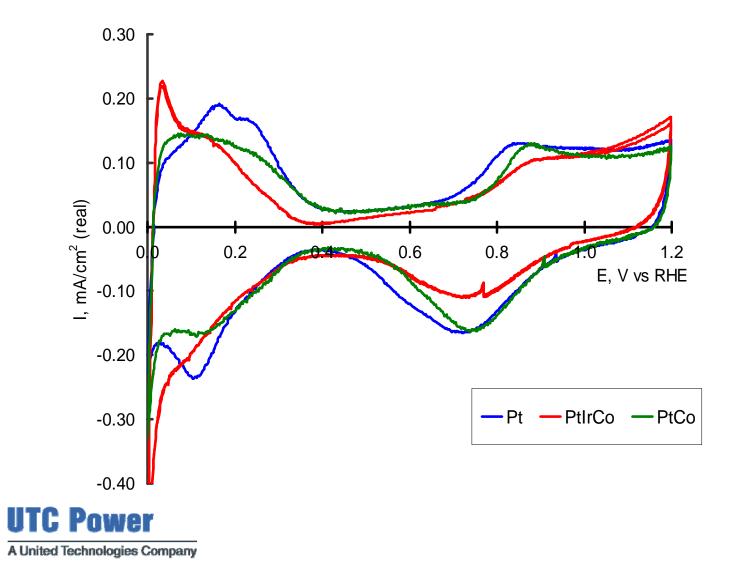


#### HIGHLY DISPERSED ALLOY CATALYST Understanding high performance materials





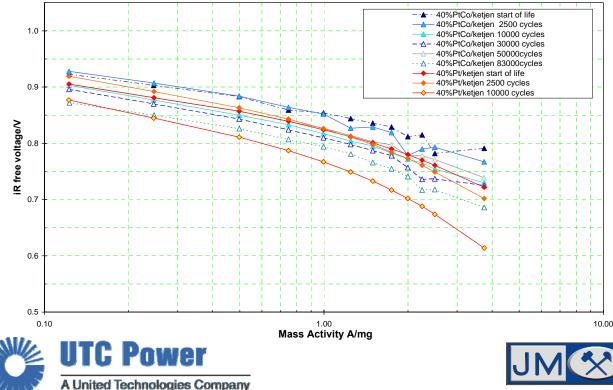
#### HIGHLY DISPERSED ALLOY CATALYST Understanding high performance materials



### 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 0.7-0.9ViR 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

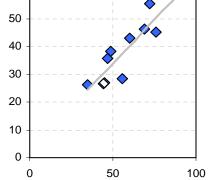


0.5M H<sub>2</sub>SO<sub>4</sub>, 363K, 24 hrs

70

60

Co leached/%



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

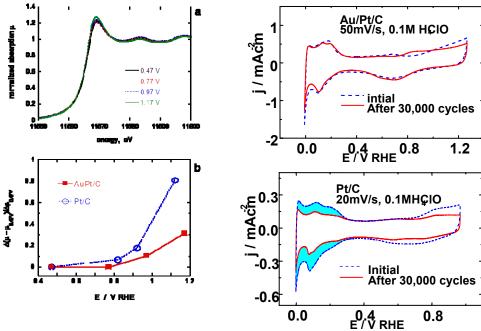
Ex-situ acid leaching PtCo alloys shows Co removal strongly dependent on surface area/particle size



#### HIGHLY DISPERSED ALLOY CATALYST Model systems to develop understanding

Segregation of Au in AuNi micropowder x-ray diffraction 1.2x10 Intensity (a.u.)  $8.0 \times 10^{3}$  $4.0 \times 10^{3}$ 0.0 24 30 36 42 Two Theta (degrees) EDS of a Pt<sub>MI</sub> /Au/Ni nanoparticle in nano-probe mode 160 – Ni ---- Au - Pt 120 Pt Intensity (Counts) 80 Ni 40 6 Distance (nm) A United Technologies Company

Learning from stabilization effects of Au clusters on Ptno 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.

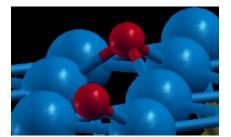


### HIGHLY DISPERSED ALLOY CATALYST Modeling to understand materials

METHODS Computational chemistry methods help to understand catalytic activity and metal dissolution

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





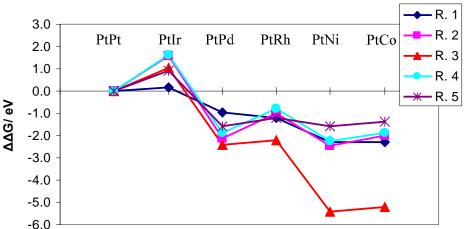
Oxygen attachment to atoms on the metal surface is the first step in the dissolution process



We calculate:

$$\Delta \Delta \mathbf{G}_{\mathsf{rxn}i} = \Delta \mathbf{G}_{\mathsf{rxn}i} \, \mathbf{I}_{Alloy} \, - \, \Delta \mathbf{G}_{\mathsf{rxn}i} \, \mathbf{I}_{P}$$

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



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# HIGHLY DISPERSED ALLOY CATALYST

#### Program team





Catalyst fundamentals Catalyst development Verification

Catalyst development : alloys, supports, MEA Prototyping



Brookhaven National Laboratory



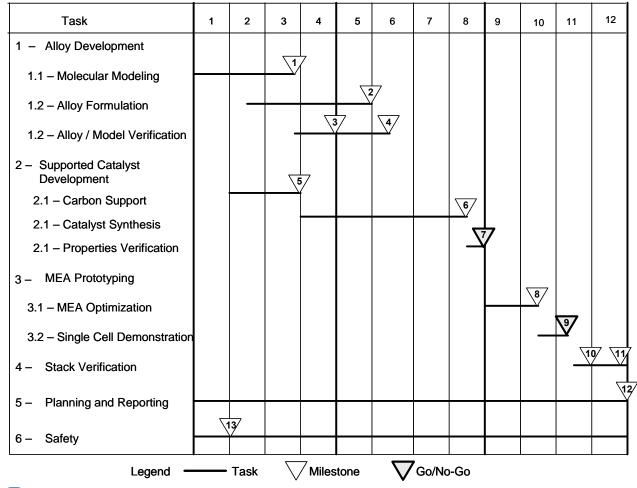
Catalyst development : supports

Catalyst fundamentals: experimental

Catalyst fundamentals: modeling



#### HIGHLY DISPERSED ALLOY CATALYST Project timeline



Project Time Period (Quarters)



# HIGHLY DISPERSED ALLOY CATALYST Program budget (total program)

| GFY '07 | \$2,214,267 |
|---------|-------------|
| GFY '08 | \$2,868,363 |
| GFY '09 | \$2,736,472 |
| GFY '10 | \$669,319   |

Cost share – 25%

