New Electrocatalysts for Fuel Cells

Principal Investigator: Philip N. Ross, Jr.

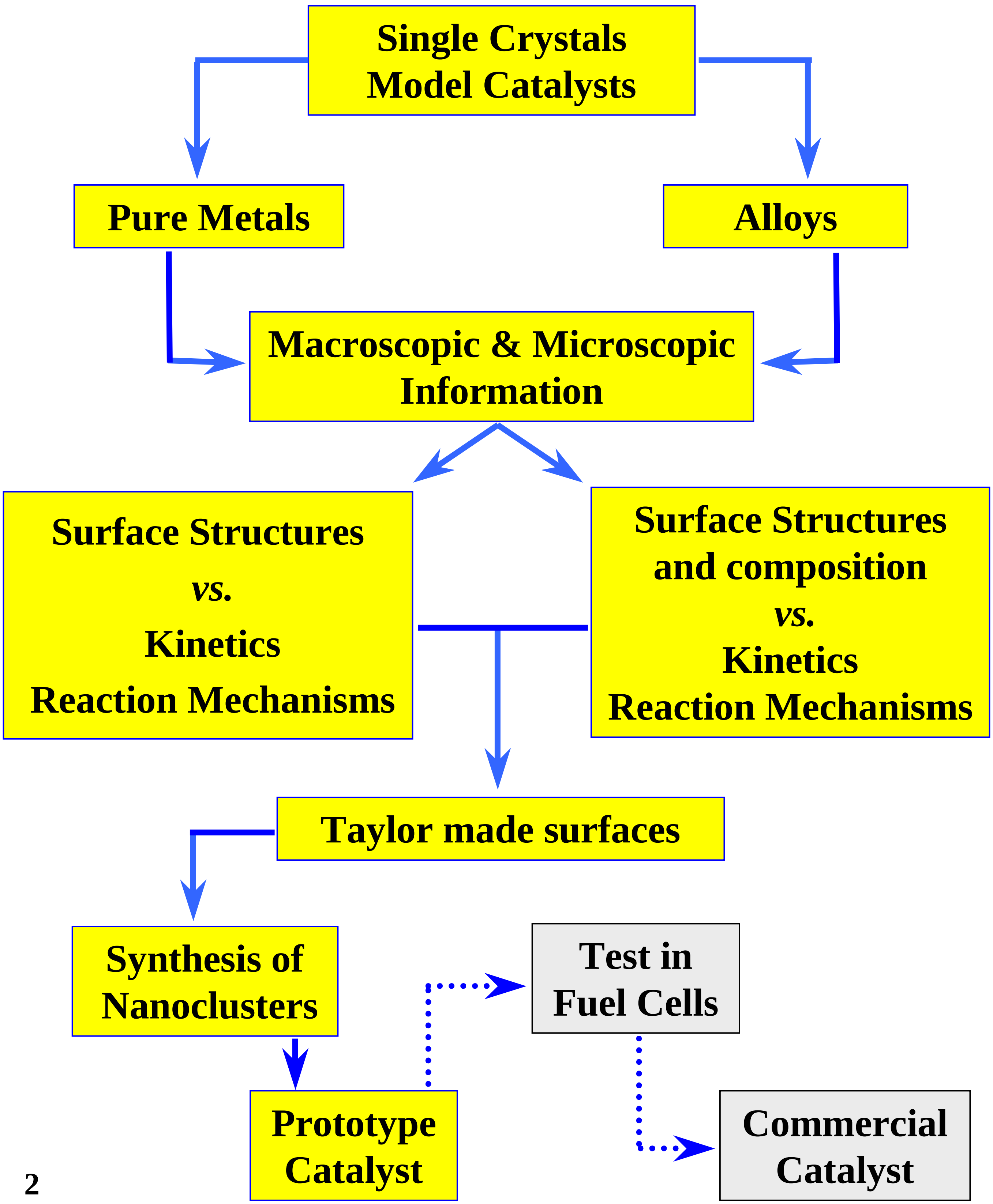
Staff Scientist: Nenad M. Markovic

Post Doctoral Fellow: Thomas J. Schmidt

Visiting Scientist: Vojislav Stamenkovic

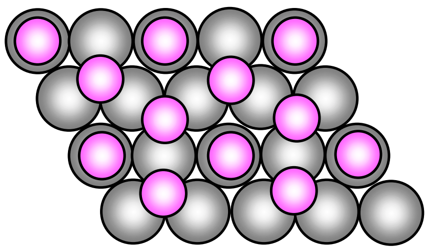
A research program conducted at the Lawrence Berkeley National Laboratory for the Assistant Secretary for Conservation and Renewable Energy, Office of Transportation Technologies, Electric and Hybrid Propulsion Division of the U.S. Department of Energy under contract No. DE-AC03-76SF00098

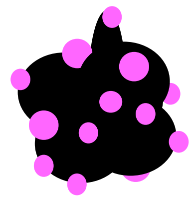
Materials-by-Design Approach

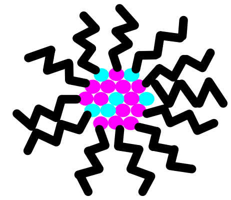


Materials-by-Design Approach

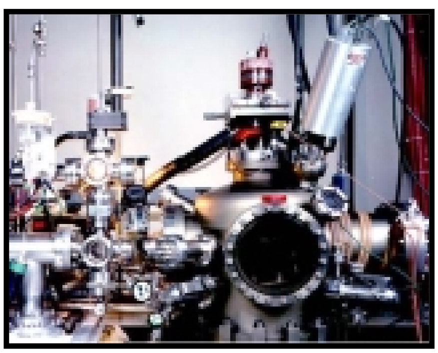
well-defined system ↔ **Fuel cell catalyst**



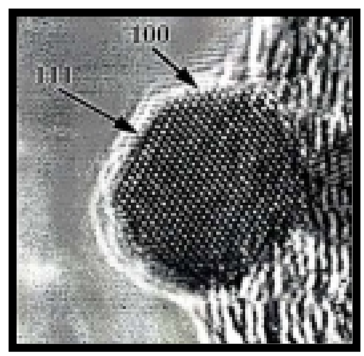




Characterization techniques

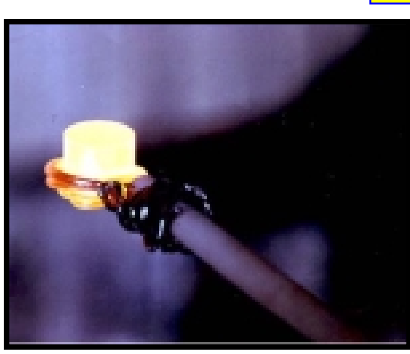


LEIS, XPS, AES, LEED

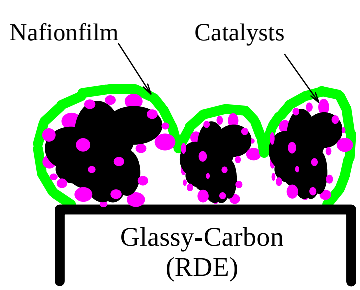


HRTEM, XRD

Kinetics



HOR, ORR, CO Tolerance



HOR, ORR, CO Tolerance

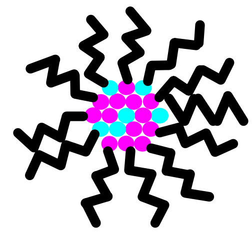
New Synthesis Pathways *via* Colloidal Precursor

Borate Reduction Pathway

$PtCl_2 + RuCl_3 + N(oct)_4[Bet_3H]$

$\Downarrow$

$PtRu[N(oct)_4Cl]_8 + 5\ Bet_3 + 2.5\ H_2$

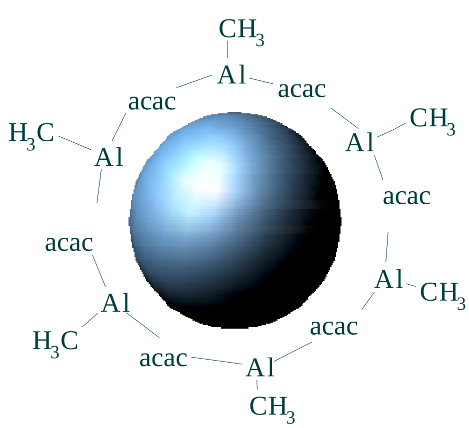


Organoaluminum Pathway

$Pt(acac)_2 + Ru(acac)_3 + 8\ Al(me)_3$

$\Downarrow$

acac = acetyl acetonate

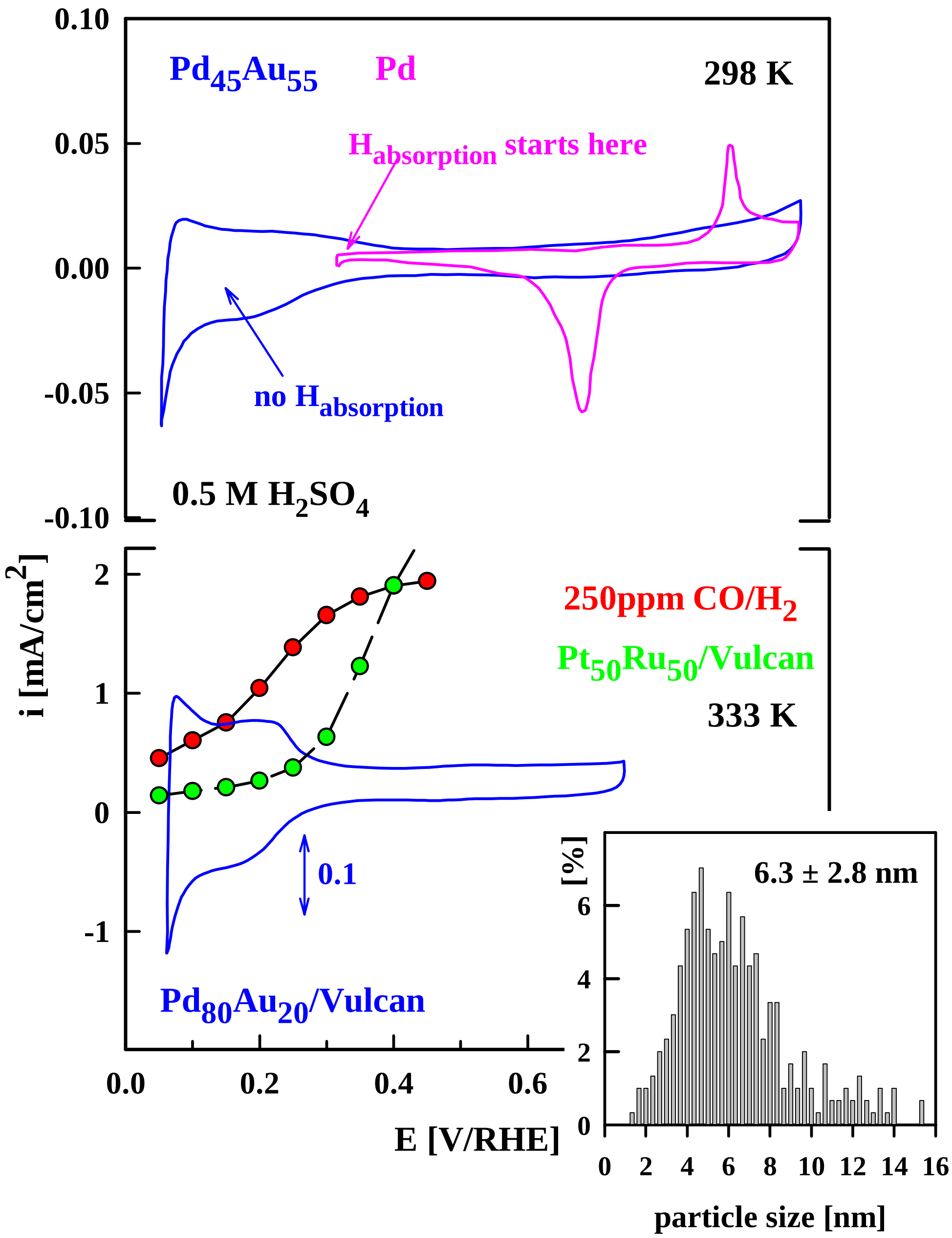


---

adsorption on high-surface area support

removal of the stabilizer → **catalyst**

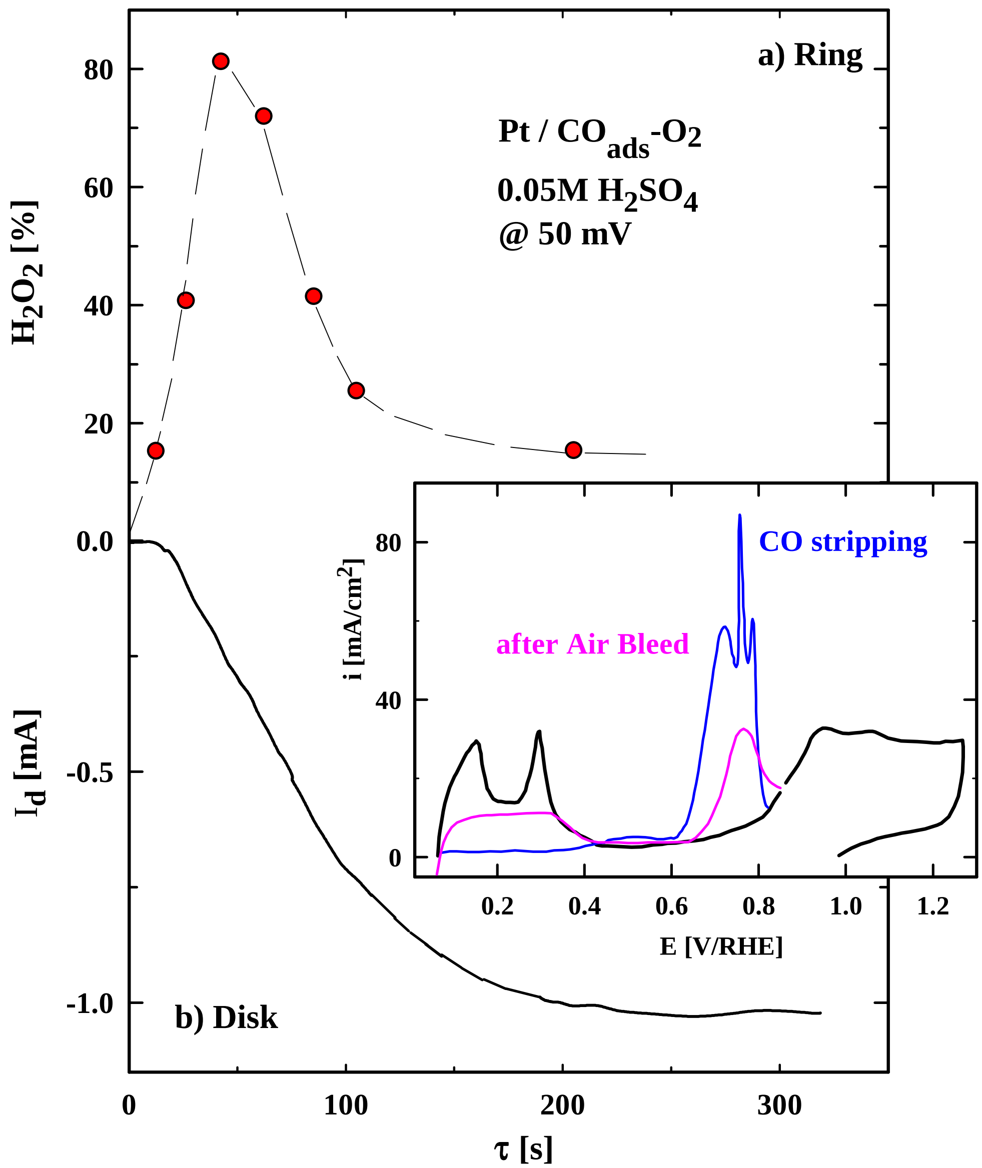
New Class of Catalyst: PdAu-Alloys



- Au stabilizes Pd: no H-absorption
- at low E: 3-5 times more active for CO/H_2 than PtRu
- promising results on non-optimized system!

Insights into ‘Air-Bleed’: 1. Pure Platinum

Air Bleed **≡ Anode catalyst cleansing by oxidative CO removal**

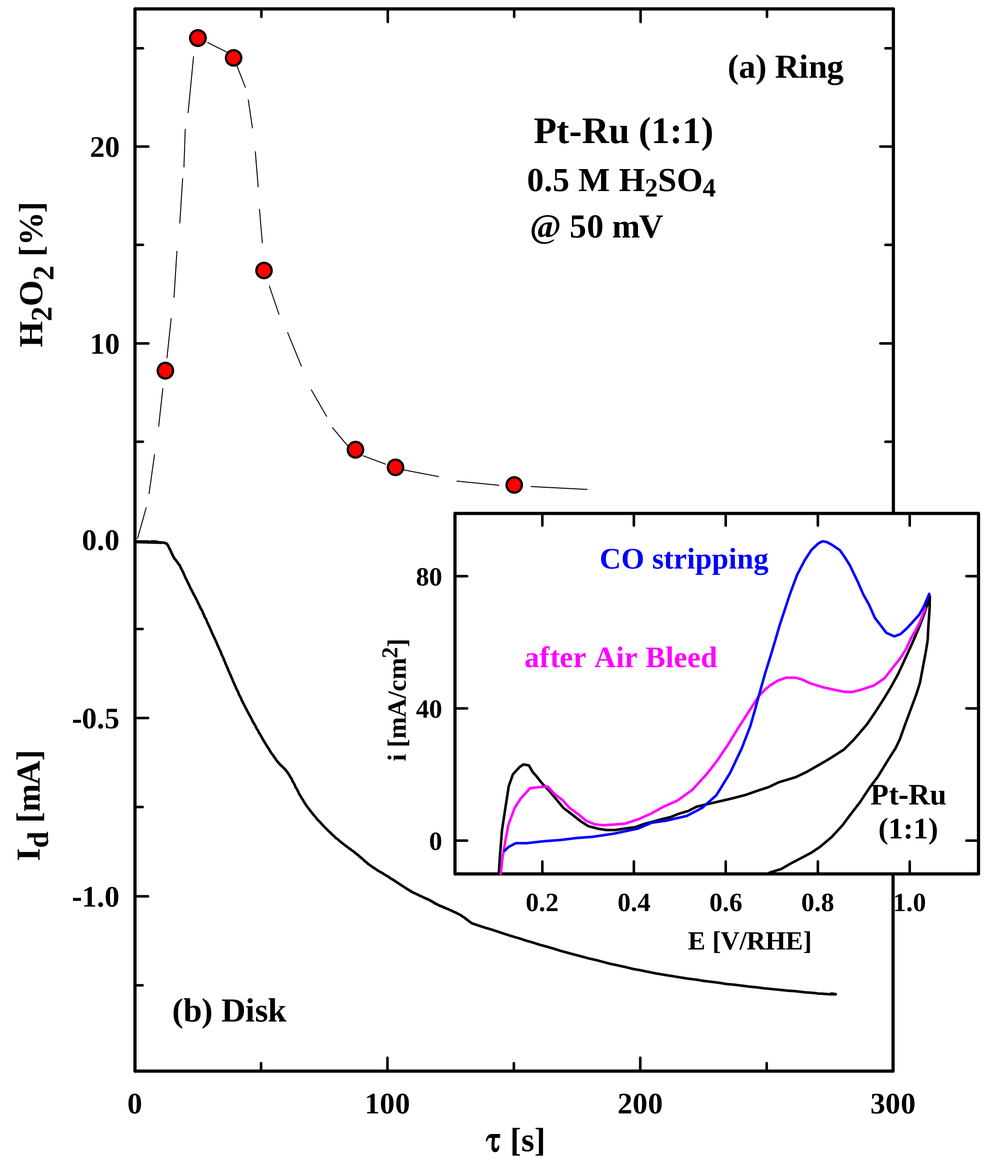


Experiment:

ORR at 50mV on CO pre-covered surface

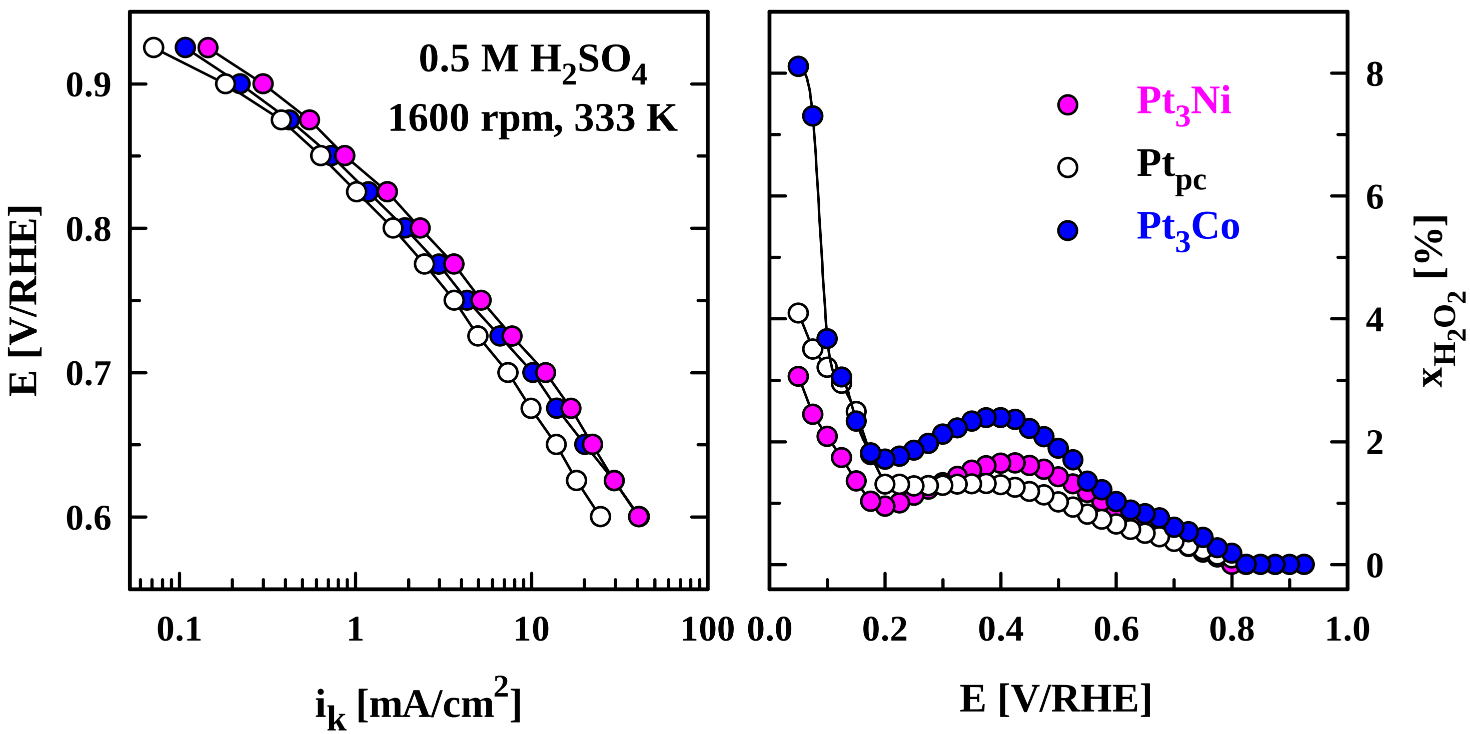
- **After air-bleed: 35 - 40 % of CO *remains* on the surface**
- **On Pt: initially ca. 80 % H_2O_2 formation**
- **at I_{diff} ca. 20% H_2O_2 (only 5-10% on CO free Pt)**

Insights into 'Air-Bleed': 2. PtRu-Alloys



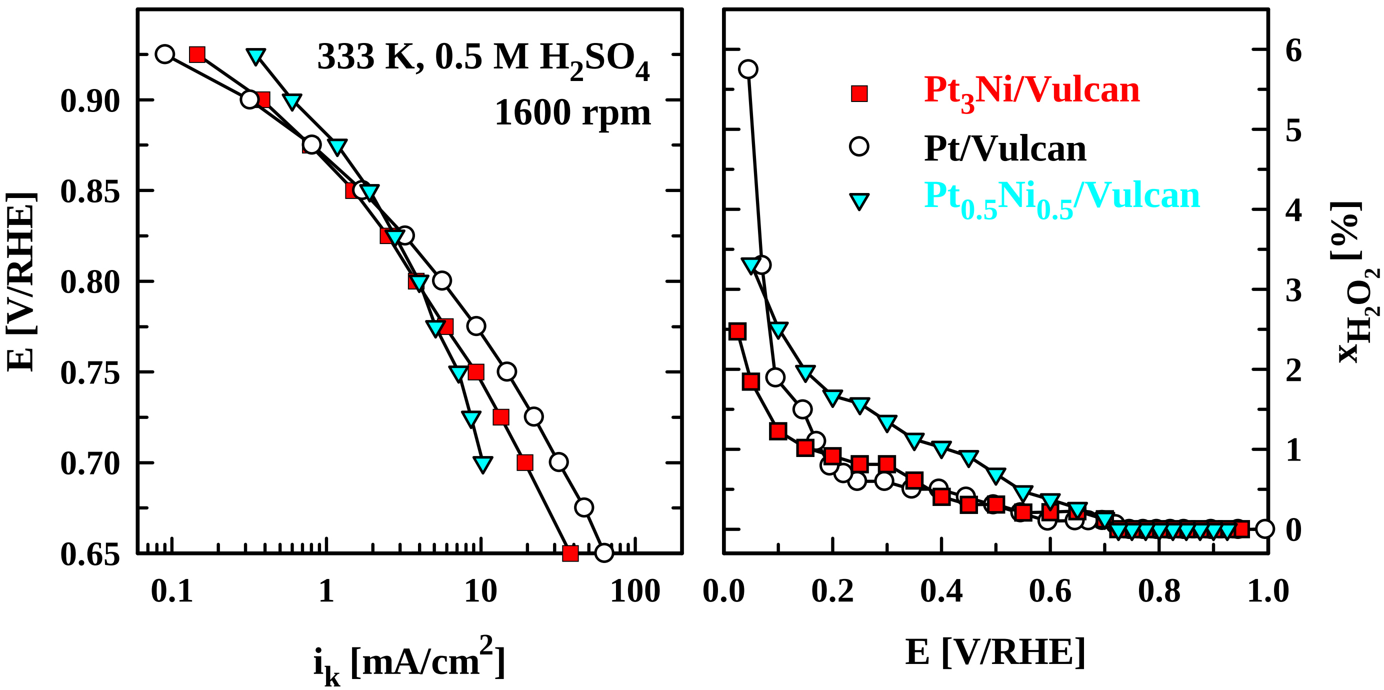
- After air-bleed: 35 - 40 % of CO *remains* on the surface
- On PtRu: initially ca. 25 % H_2O_2 formation
- at I_{diff} ca. 5 % H_2O_2 (similar to CO free surface)
- *H_2O_2 effects on membrane stability?*

PtNi and PtCo Alloys for Oxygen Reduction
1. Well-Defined Alloy Electrodes

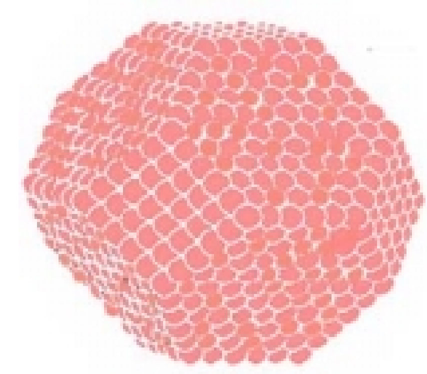


- **UHV-prepared and characterized: AES, LEIS**
- **Activity at 333 K: Pt_3Ni > Pt_3Co > Pt**
- **Similar small amounts of H_2O_2 on all three surfaces**

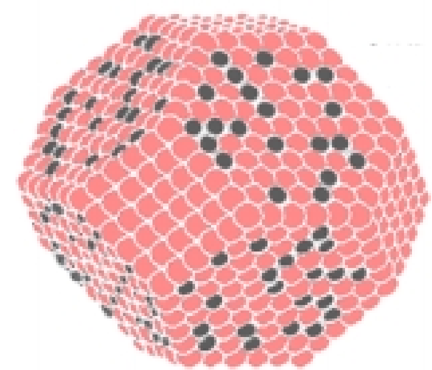
PtNi-Alloys for Oxygen Reduction
2. High-Surface Area Catalysts



Pt



PtNi



Pt substitution

- **Similar activities at 333 K for PtNi/C and Pt/C**
- **Similar small amounts of H_2O_2**
- **Possibility to decrease amount of Pt in FC catalyst**

Milestones

Anode Side

- **Pt-FREE CATALYST**
  - **PdAu-Alloys with high CO-tolerance**
- **AIR-BLEED**
  - **Insights into mechanism (*e.g.*, H_2O_2 formation)**

Cathode Side

- **Pt SUBSTITUTION**
  - **Pt_3Ni and Pt_3Co with similar activity as Pt**

Future Research

Anode Side

- Optimization of PdAu catalysts
  - Stoichiometry and particle size
- Electrocatalysis on Pd thin metal films
  - Electronic effects
  - Select the most promising substrate for the Pd thin film electrode concept
- Simulation of ‘Air-bleed’
  - on FC catalysts under FC conditions

Cathode Side

- Optimization of PtNi and PtCo catalysts
  - Stoichiometry
  - Minimization of Pt amount
  - Pt-skin effects (electronic modification of Pt)
  - Anion effects
- New class of ORR catalysts

Collaborations

Industry

- E-Tek, New Jersey, NJ, USA
- Honda, Japan
- 3M, Minneapolis, MN, USA
- TJ Technology, Detroit, MI, USA

Universities and Institutes

- Max-Planck-Institut fuer Kohlenforschung, Muelheim/Ruhr, Germany
- University of Ulm, Germany
- Paul-Scherrer-Insitut, Villigen, Switzerland
- Universidad d'Alicante, Spain
- Texas Tech University, Lubbock, TX, USA
- Lawrence Berkeley National Laboratory, Somorjai-Group, Berkeley, CA, USA