Neutrons Role in Chemistry and Catalysis Studies?

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Neutrons for Catalysis and Chemistry in Nanostructured Materials

Advantages:

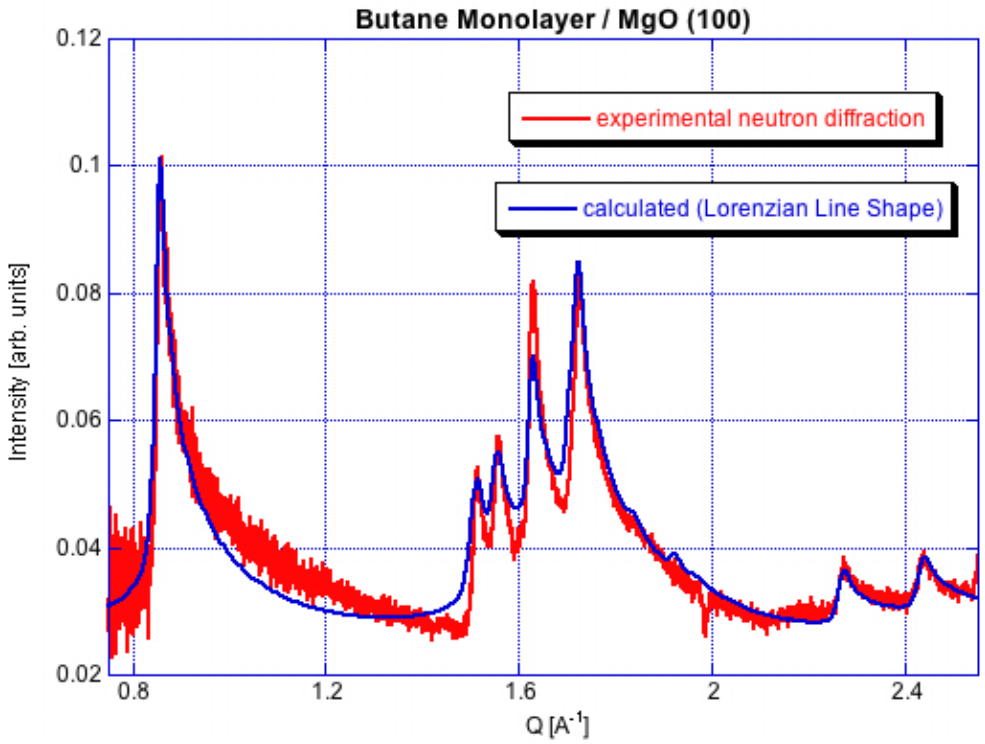
- ✓ *Neutrons are highly penetrative and samples can be contained in stainless steel and quartz cells allowing the performance of experiments at high pressure and temperatures (in situ studies)*
- ✓ *Neutrons do not stimulate chemistry as do electrons and photons used in many other techniques.*

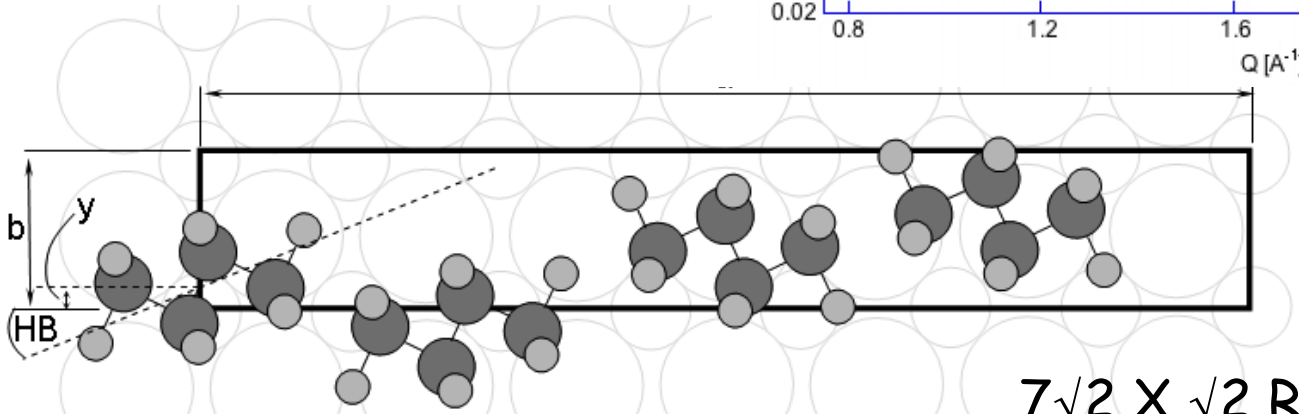
Applications:

- **Structure of Nanocatalysts:**
  - ✓ **Local disorder in crystalline materials (ideal for systems lacking long range order)**
  - ✓ **Particle size distribution**
  - ✓ **Structure of molecules containing low Z atoms**
- **Dynamics of reactions and transformation of adsorbed species on heterogeneous catalysts under reaction conditions.**
- **Catalytic mechanisms.**
- **Chemistry of paramagnetic molecules and sites.**
- **Catalyst deactivation / poisoning and reaction intermediates.**

Neutrons Ideally Suited to Characterize Molecular Film Structure on Nanoparticles

Neutron Diffraction used to determine that monolayer butane (C_4D_{10}) films form a 7√2 X √2 R45° commensurate solid on MgO(100) surfaces

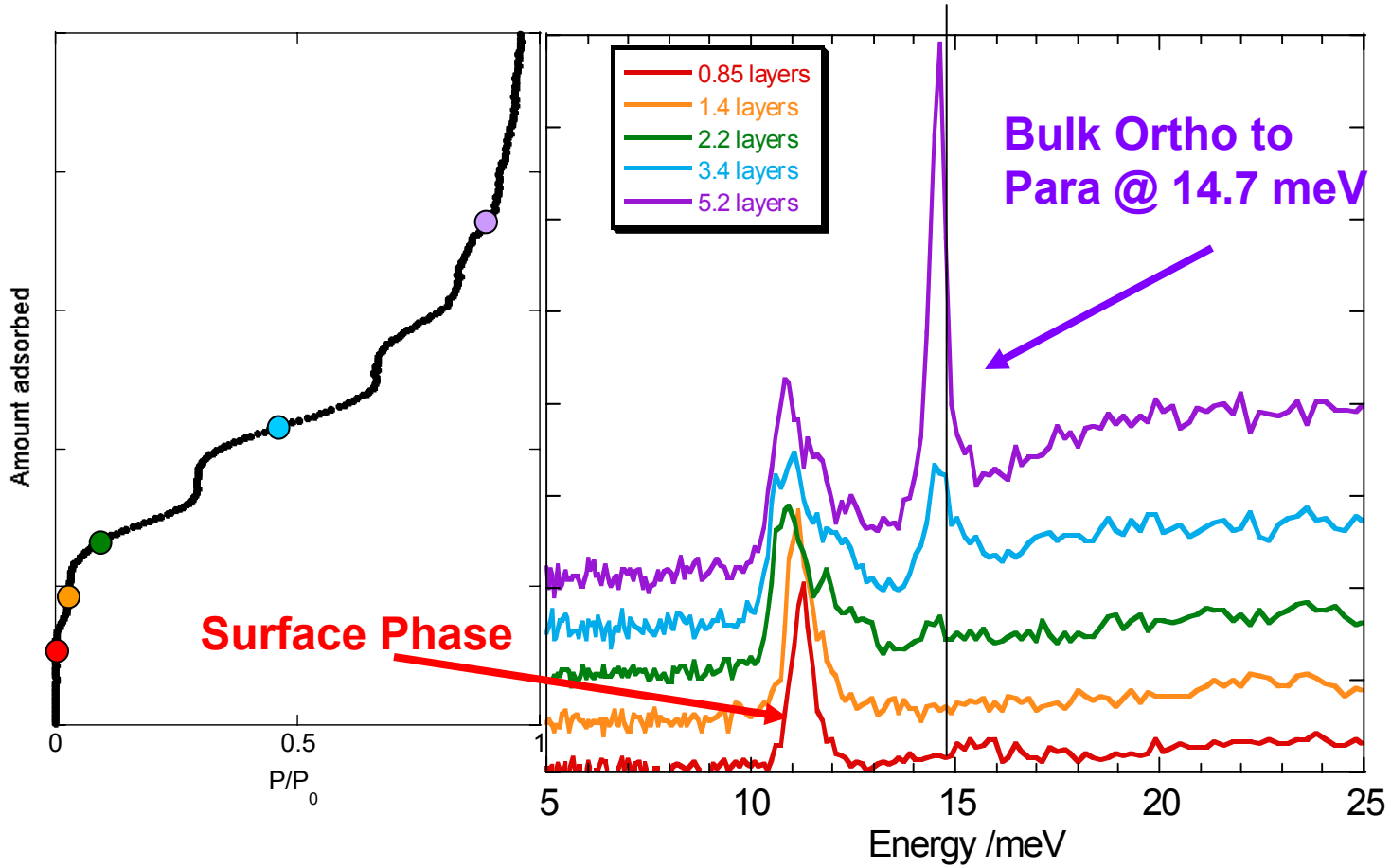




7√2 X √2 R45°

S. Channa, R. Cook, T. Arnold, S. Clark, J.Z.Larese
ORNL UTK ISIS Cambridge Univ.

Hydrogen Dynamics on Clean and Metal Cluster Decorated Particles

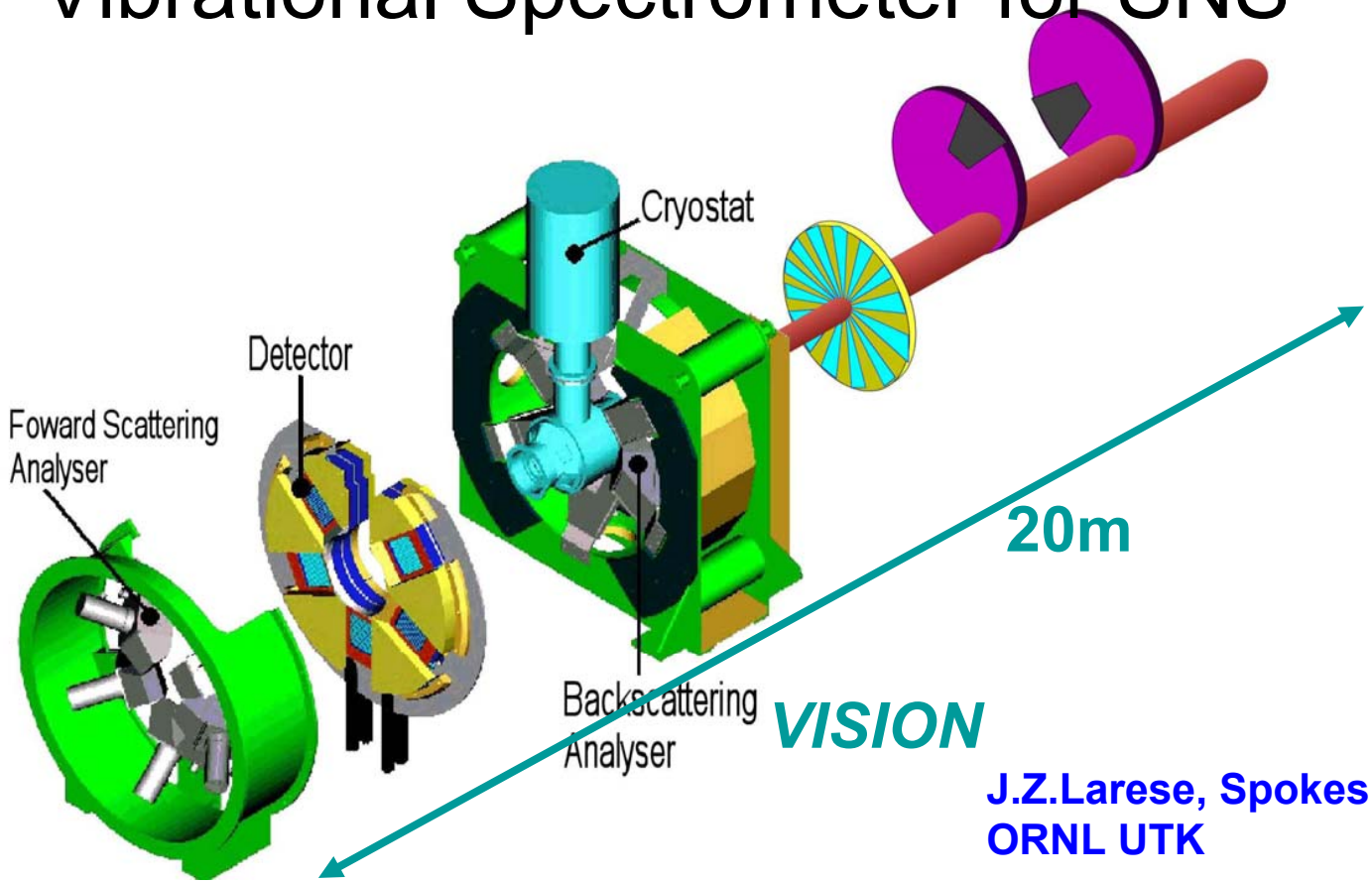


Ortho-to-para transition can be used to measure rotational barrier height and Potential Energy Surface of H_2 Metal Oxide Interaction

L. Frazier,T. Arnold, A. Ramirez, R. Hinde, J.Z.Larese ORNL UTK ISIS

VISION

Vibrational Spectrometer for SNS

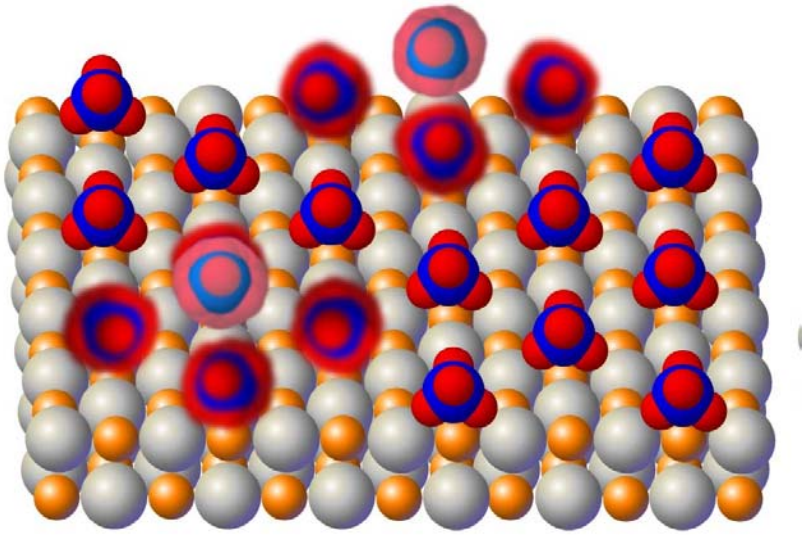


J.Z.Larese, Spokesperson
ORNL UTK

- VISION, a neutron analogue of an IR/Raman Spectrometer and ideally suited for probing vibrational dynamics of molecular species while simultaneously providing structural information

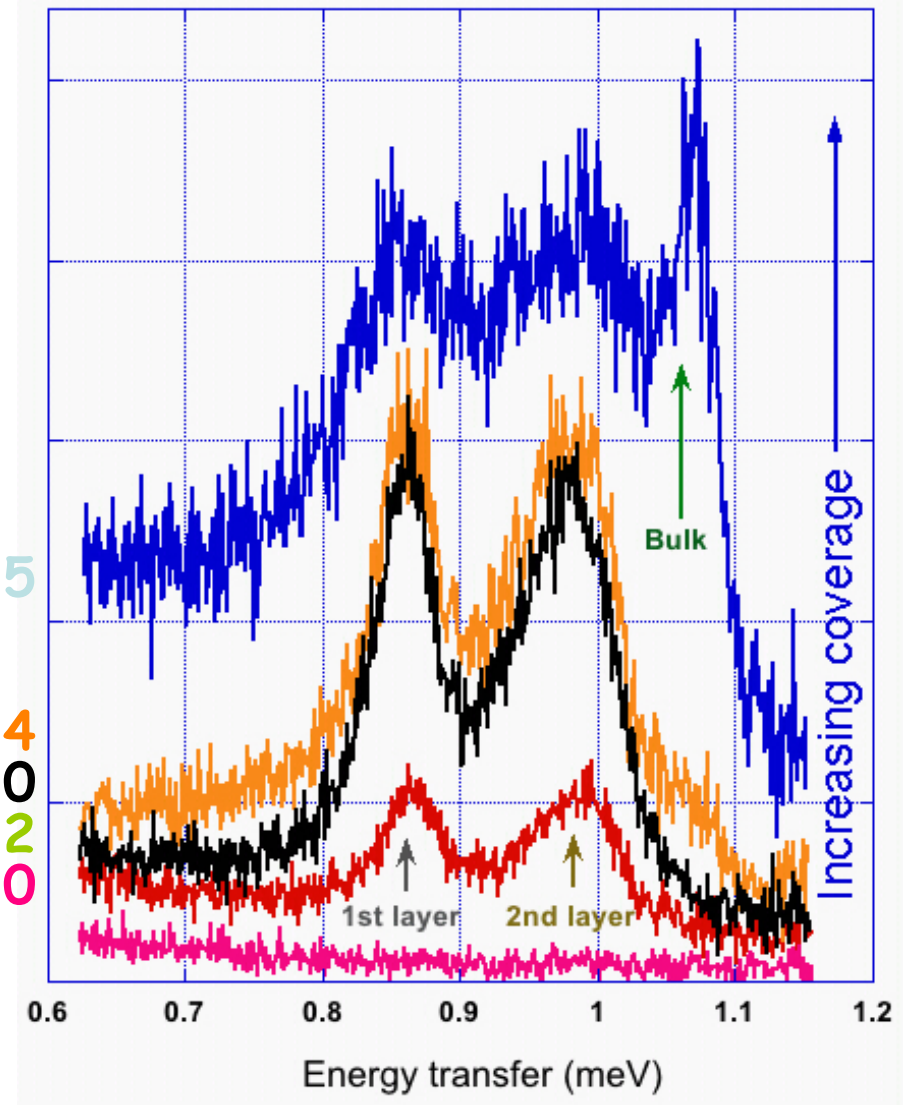
Student Training/Involvement

Adsorbed Films on Nanoparticles

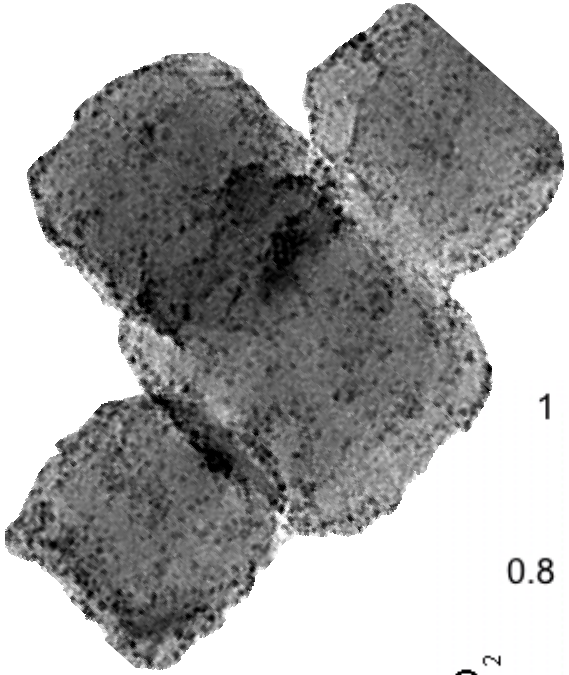


Neutrons are powerful probes of the structure and dynamics of adsorbed molecular films on nanoparticle surfaces and interfaces

J.Z.Larese, D. Martin, CJ Carlile, M Adams
ORNL, UTK, ISIS, Univ. Madrid

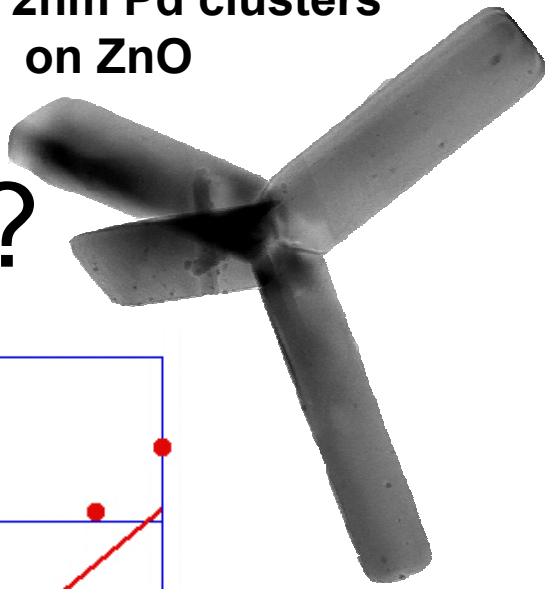


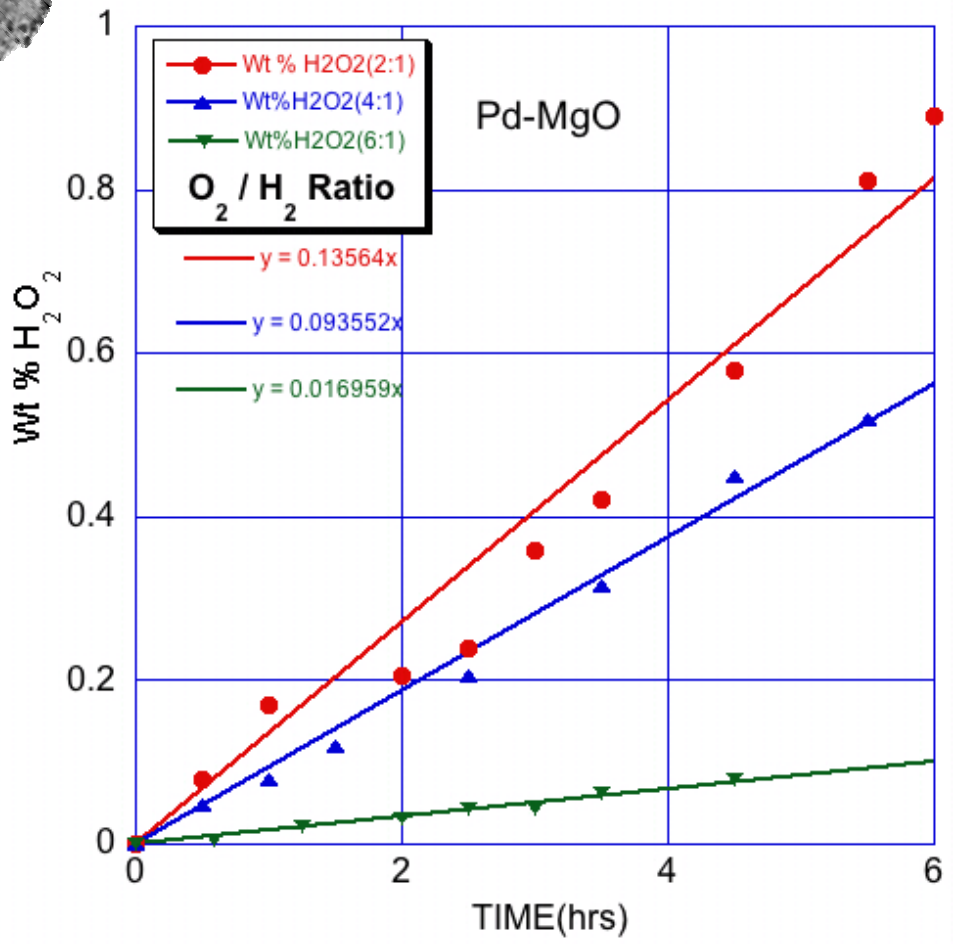
Last Minute?



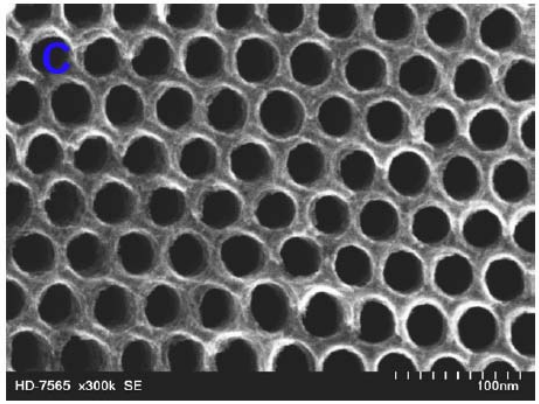
2nm Pd clusters on MgO

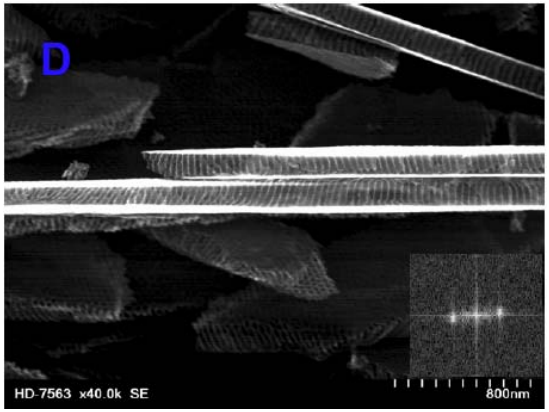
2nm Pd clusters on ZnO

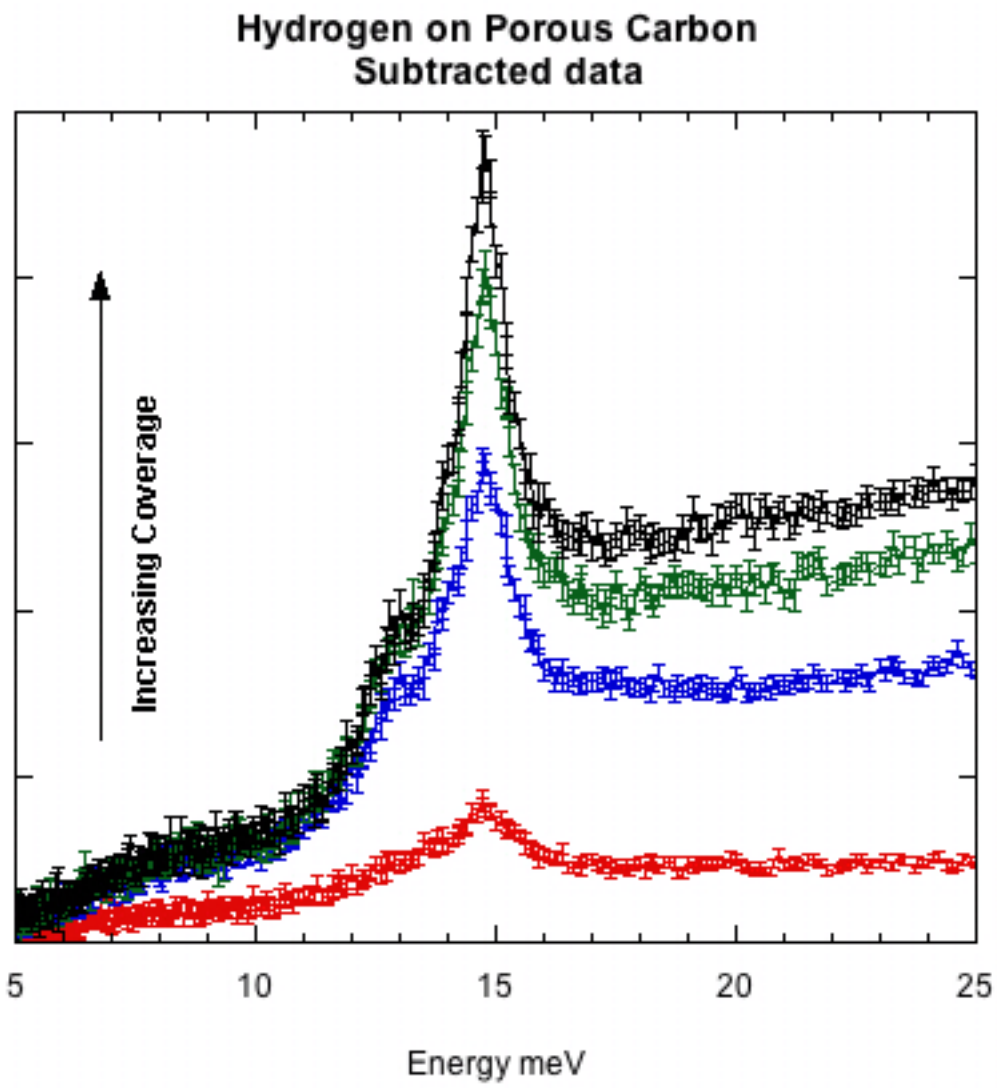




Hydrogen in carbon pores

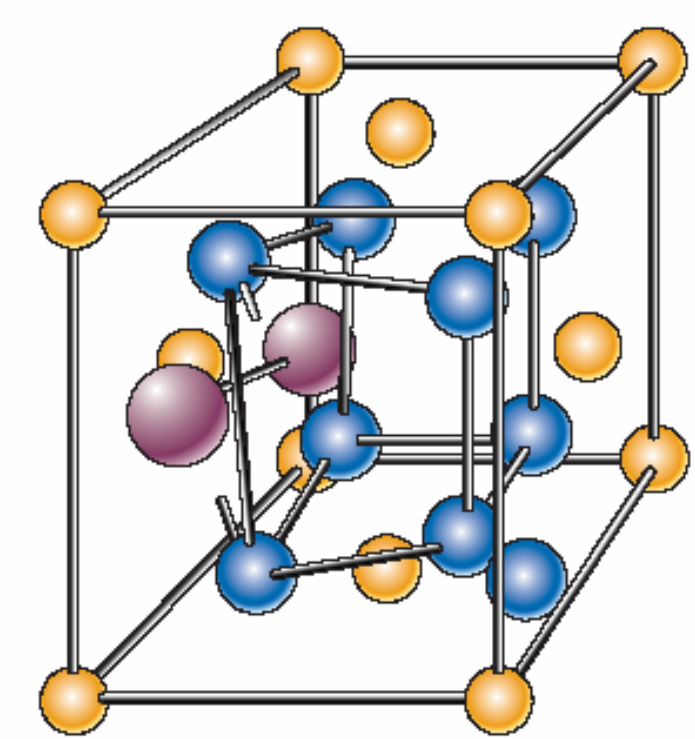


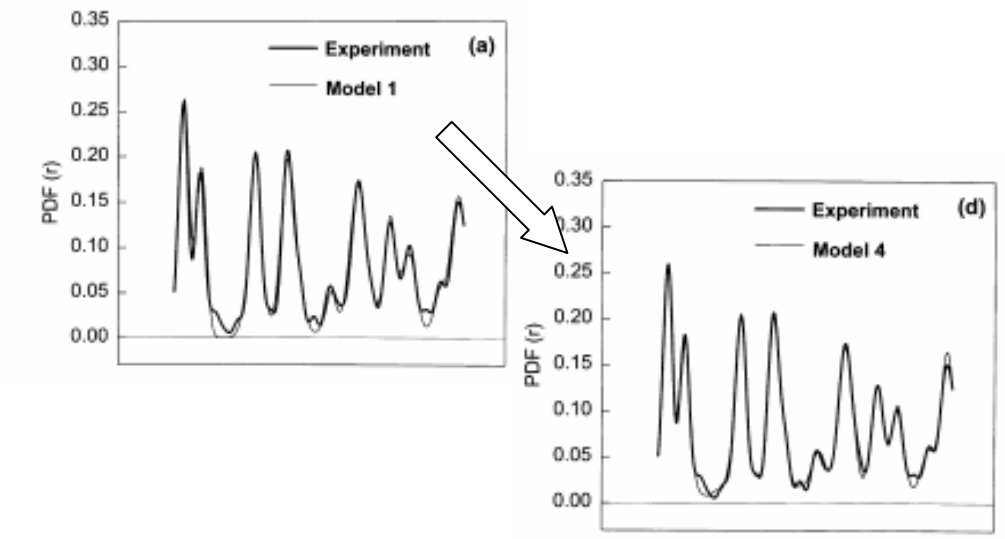




Looking at the structure of Nanoparticles

Oxygen in CeO_2 nanoparticles used in automobile catalytic converters





- Enhanced visibility of light elements with neutrons
- Statistical accuracy limits structural details discernible.

E. Mamontov, T. Egami: