CO2 Sequestration: Scientific Opportunities with X-Rays at the ALS

Zahid Hussain
Scientific Support Group
Advanced Light Source
Lawrence Berkeley National Laboratory

Possible CO2 Sequestration Scenarios

- Chemical reaction of CO2 with mineral surface to form stable carbonate (carbonate have lowest free energy product): e.g.,

$Mg^3Si^2O^5(OH)^4+3CO^2 = 3MgCO^3+2SiO^2+2H^2O$
(sepentine)

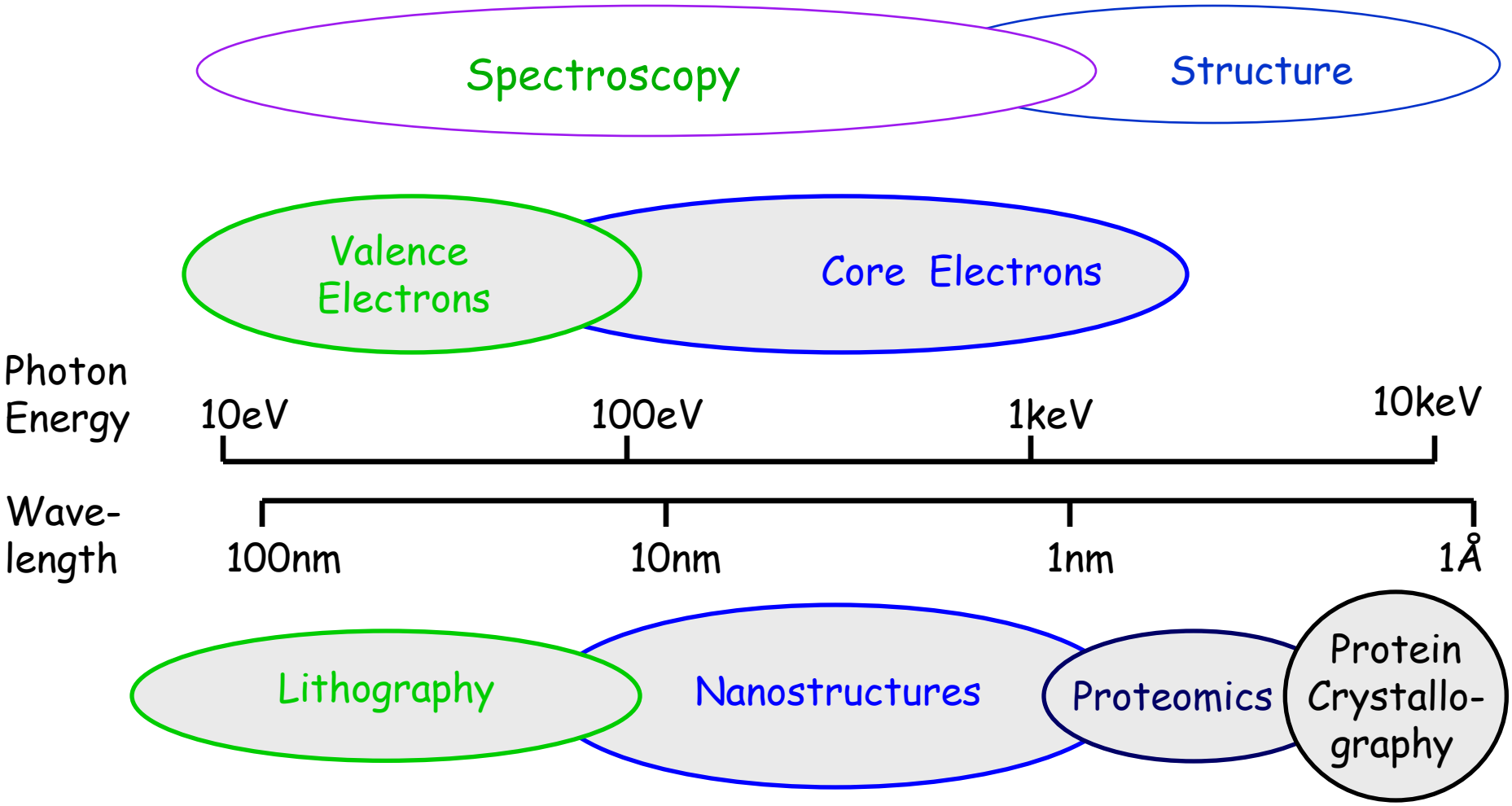
Volume change: $\delta V/V$ = ~+20%; exothermic,

$Mg^2SiO^4+2CO^2(aq) = 2MgCO^3+SiO^2$
(olivine)

Volume change: $\delta V/V$ = ~+80%; exothermic,

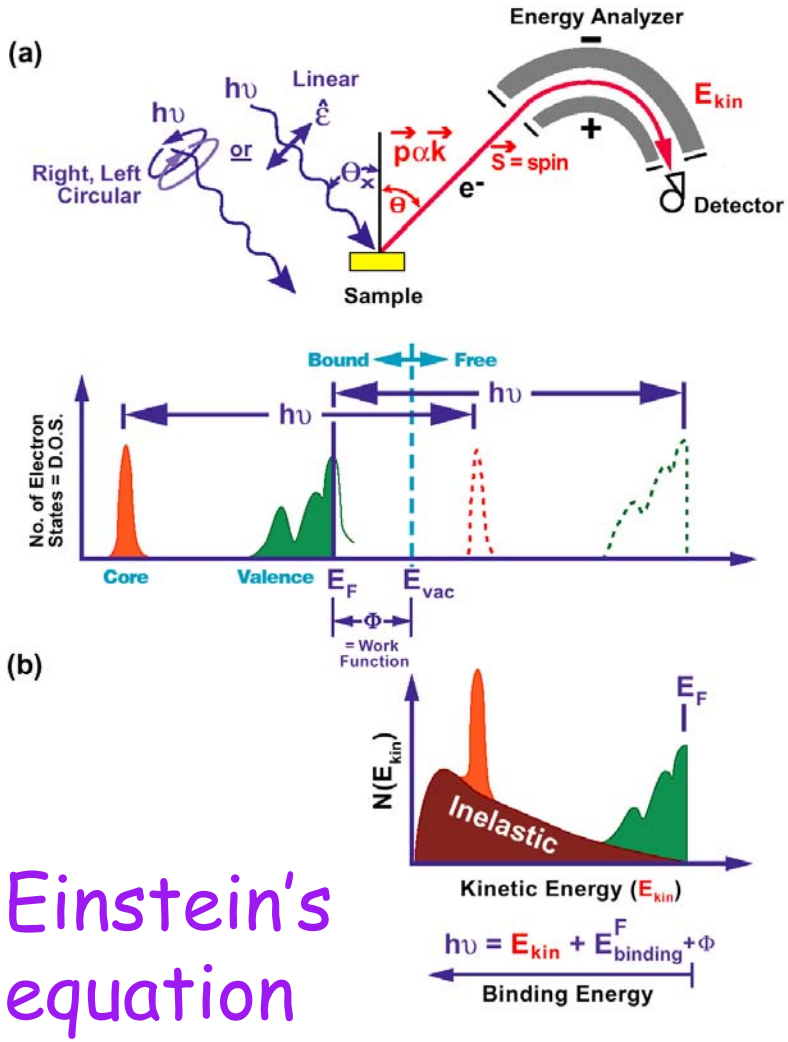
- Study in-situ electronic structure of surface chemical reactions of Co2 with rocks components, its intermediate and products using novel Ambient Pressure XPS system pioneered at ALS…….**Idea:** Courtesy Gordon Brown

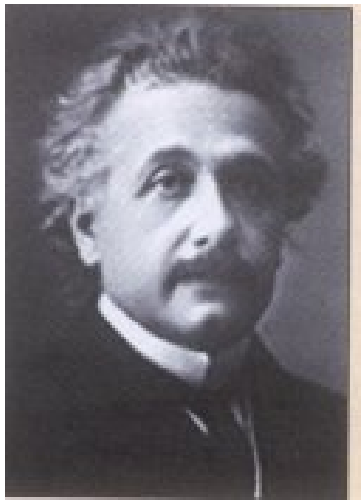
Science with Light Sources



Adopted from: Franz Himpsel, CMMP '07

Photoelectron Spectroscopy





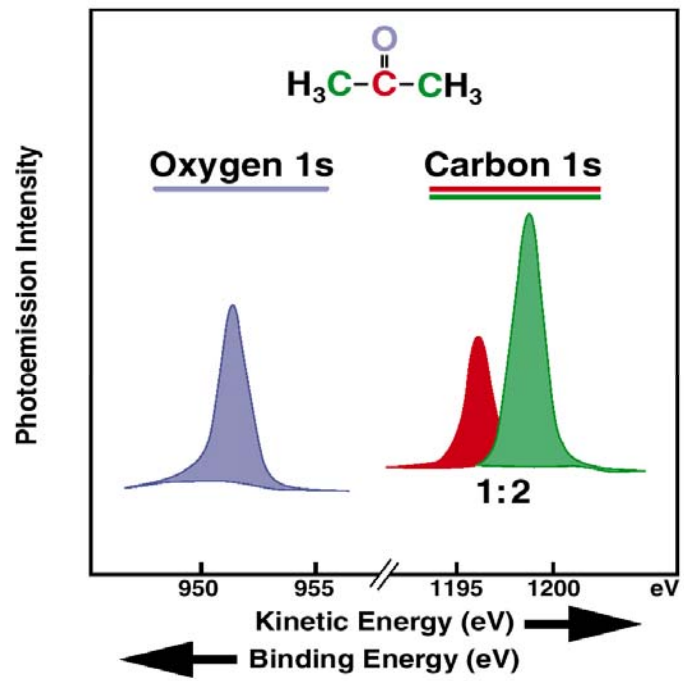
Einstein's equation

ag.zh/photospectros1/7-97

Photoemission - Core Level Spectroscopy

Provides information about

- Kind of atom
- Number of atoms
- Chemical State – simple analysis



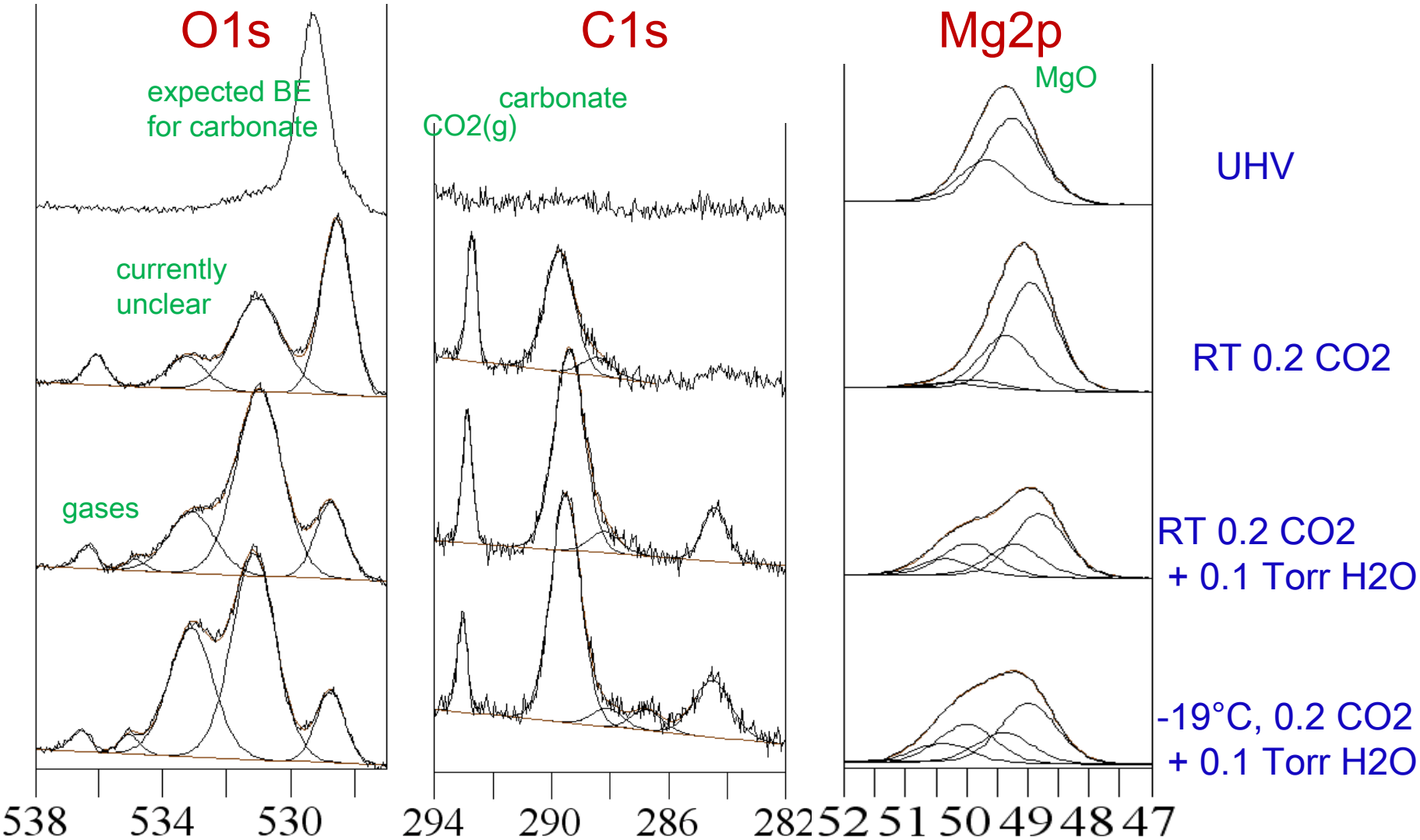
Sensitivity to Hydrogen Bonding?

(Siegbahn et al)

Lab x-ray source: Resolution = ~ 0.5 eV (mono)

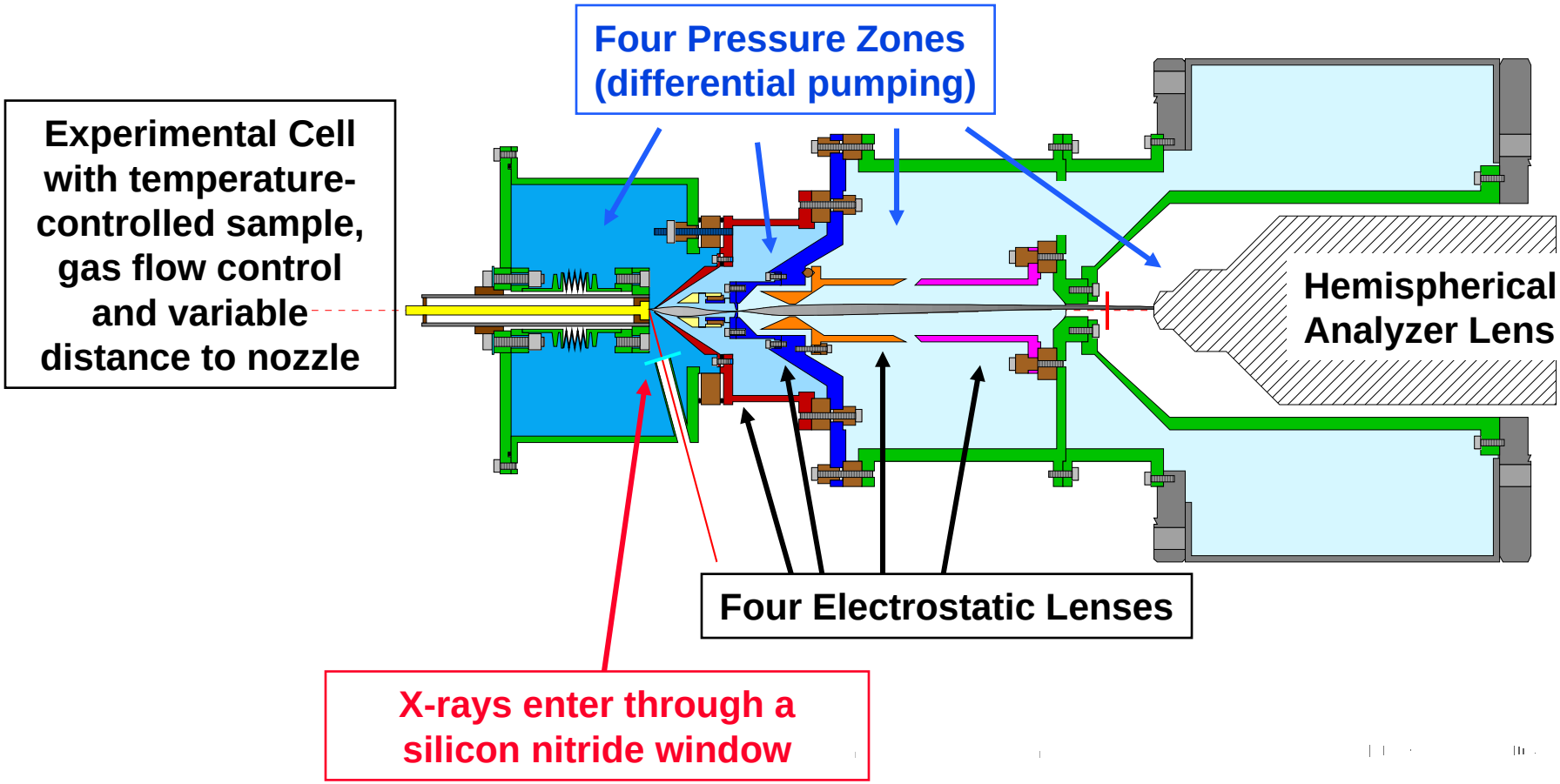
ag.zh/photospectros2/7-97

IN SITU XPS Study of CO_2 & H_2O with MgO(100)



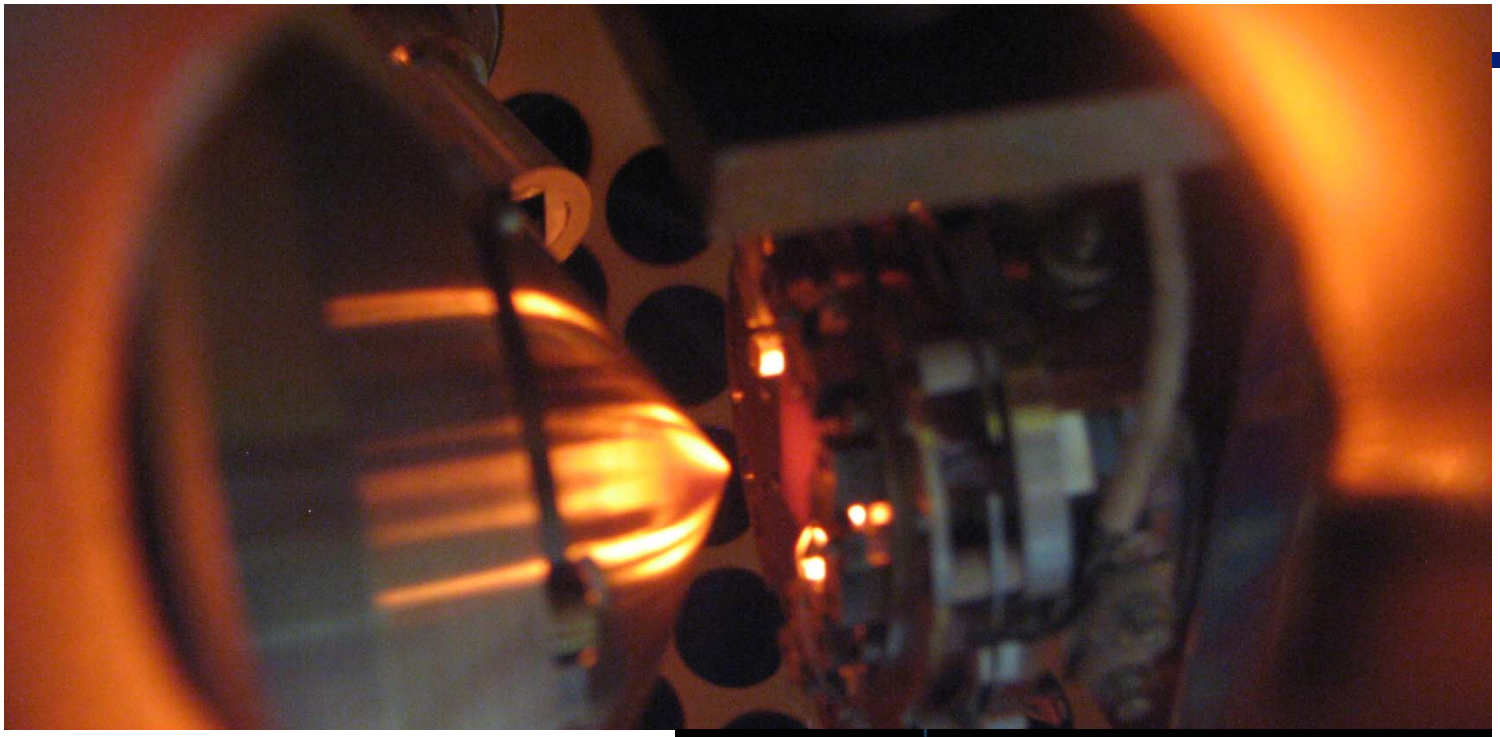
G. Brown, A. Nilsson (Stanford University), H. Bluhm (CSD) et al, 2009, Unpublished

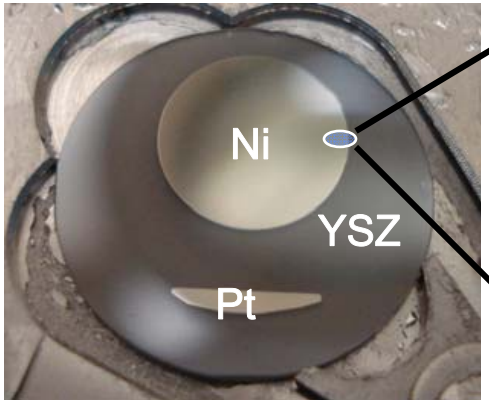
Ambient Pressure Photoemission: ~ 10 torr

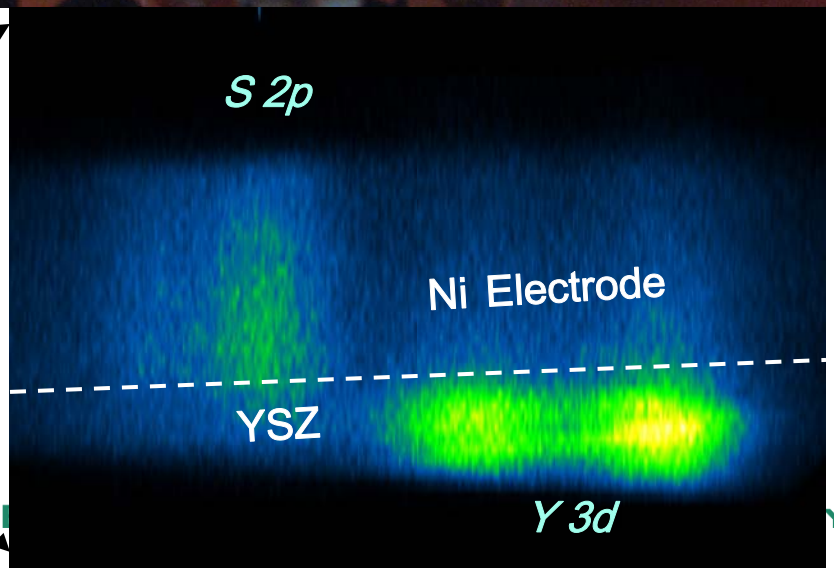


D.F. Ogletree, H. Bluhm, Ch. Fadley, Z. Hussain, M. Salmeron, Materials Sciences Division and Advanced Light Source, LBNL.

AP-XPS on Ni-YSZ-Pt fuel cell



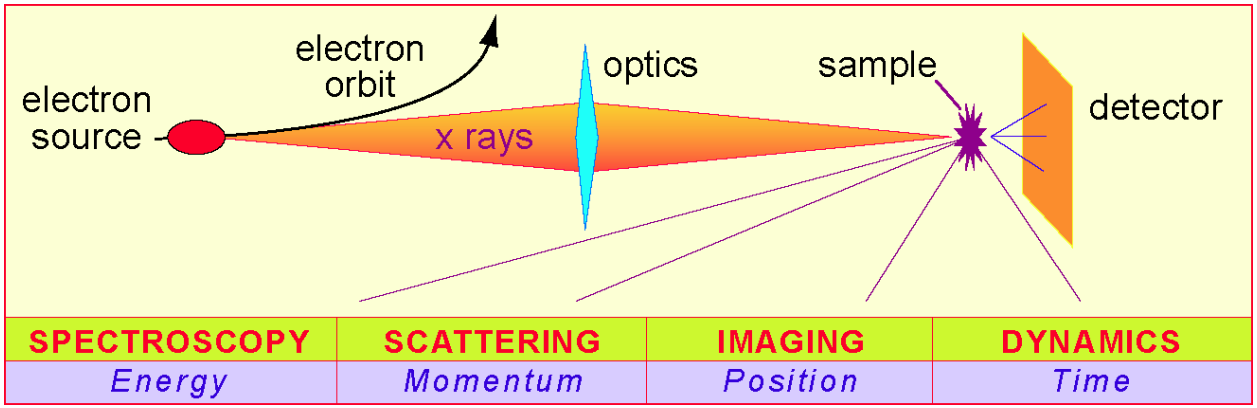




>750C

250mTorr H_2 + 250mTorr H_2O

ALS BL 9.3.2



The fundamental parameters that we use to perceive the physical world (energy, momentum, position, and time) correspond to three broad categories of synchrotron experimental measurement techniques: spectroscopy, scattering, and imaging. By exploiting the short pulse lengths of synchrotron radiation, each technique can be performed in a timing fashion.

Spectroscopy	Scattering	Imaging
01 Low-Energy Spectroscopy	05 Hard X-Ray Diffraction	09 Hard X-Ray Imaging
02 Soft X-Ray Spectroscopy	06 Macromolecular Crystallography	10 Soft X-Ray Imaging
03 Hard X-Ray Spectroscopy	07 Hard X-Ray Scattering	11 Infrared Imaging
04 Optics/Calibration/Metrology	08 Soft X-Ray Scattering	12 Lithography