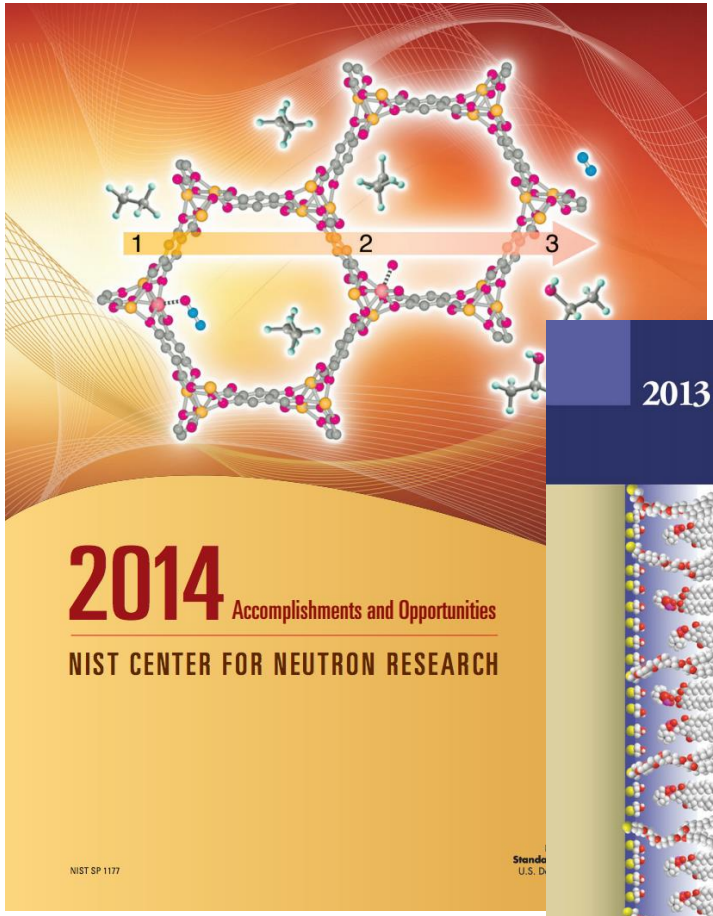
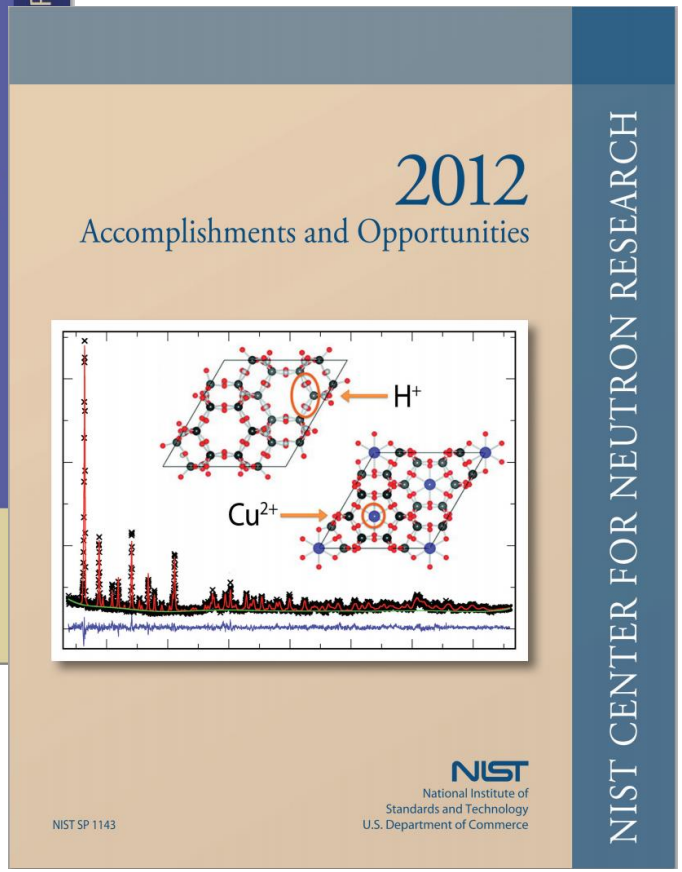
NCNR Science Highlights



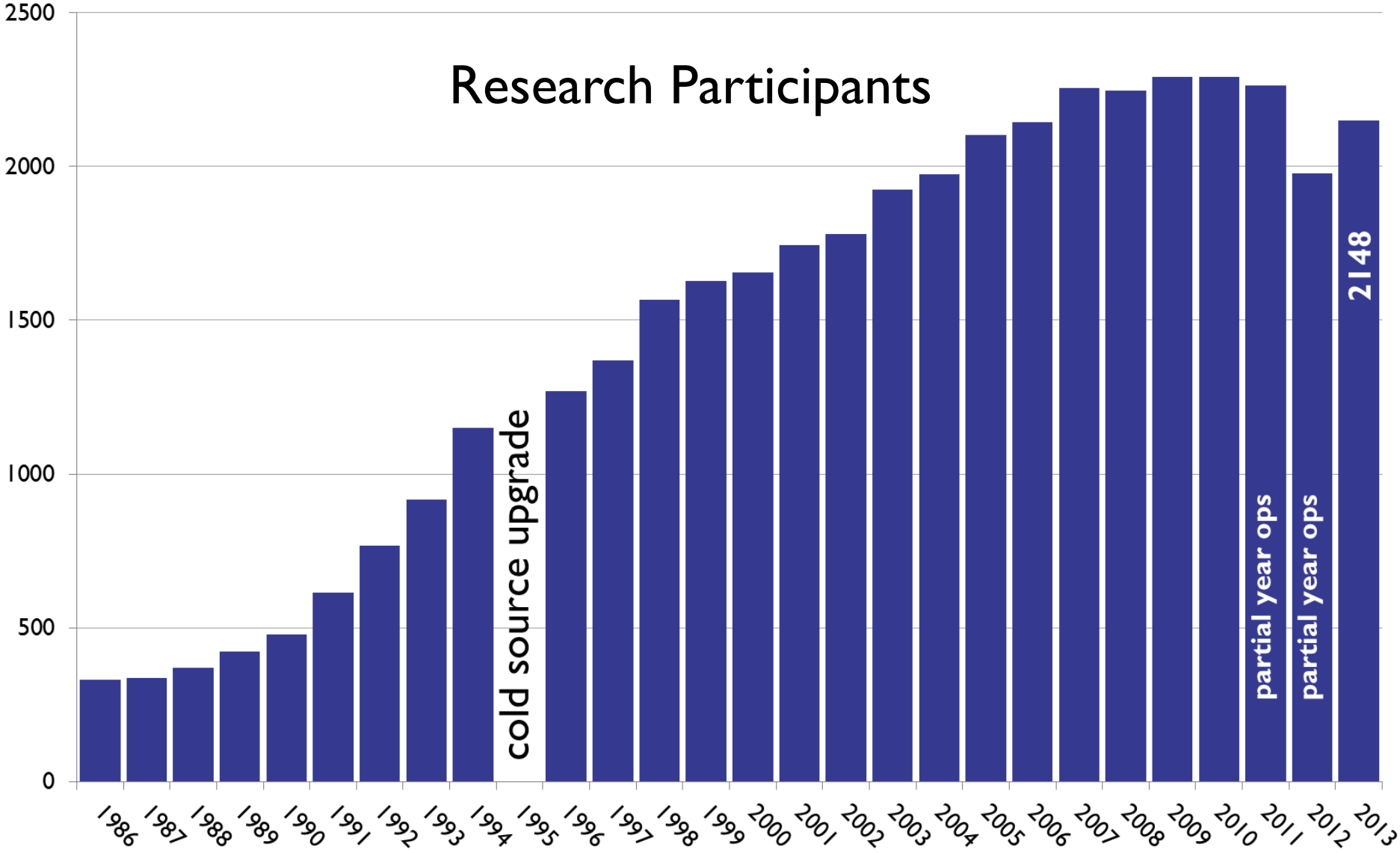


Craig Brown

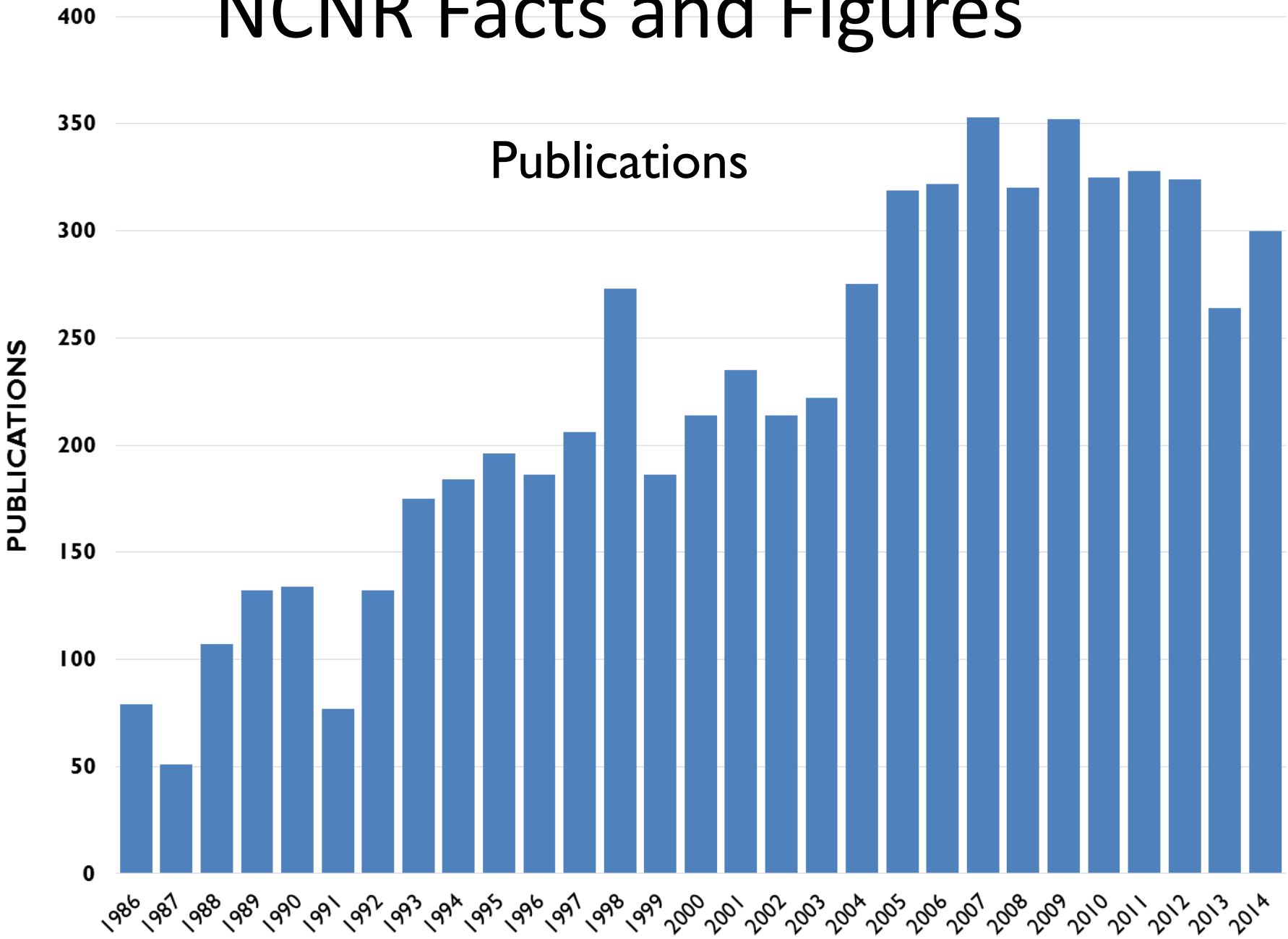
NCNR Facts and Figures

- ≈ 240 operating days/year
- ≈ 99% reactor reliability
- 28 experimental beam instruments/experiments
- ≈ 2000 research participants/year
- ≈ 300 publications/year
  - ≈ 15% in very high impact journals

NCNR Facts and Figures



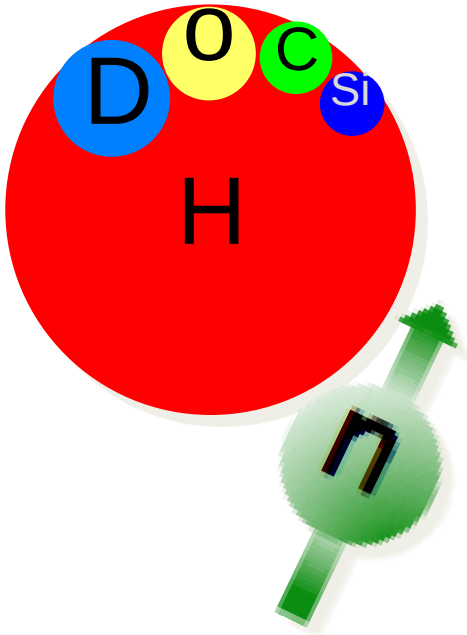
NCNR Facts and Figures



Neutron Properties

Isotopes have different scattering powers

H : 1 proton
1 electron



D : 1 proton
1 neutron
1 electron

Incoherent scatterer
- Does not ‘see’ neighbor atoms

Coherent scatterer
- ‘Sees’ neighbor atoms

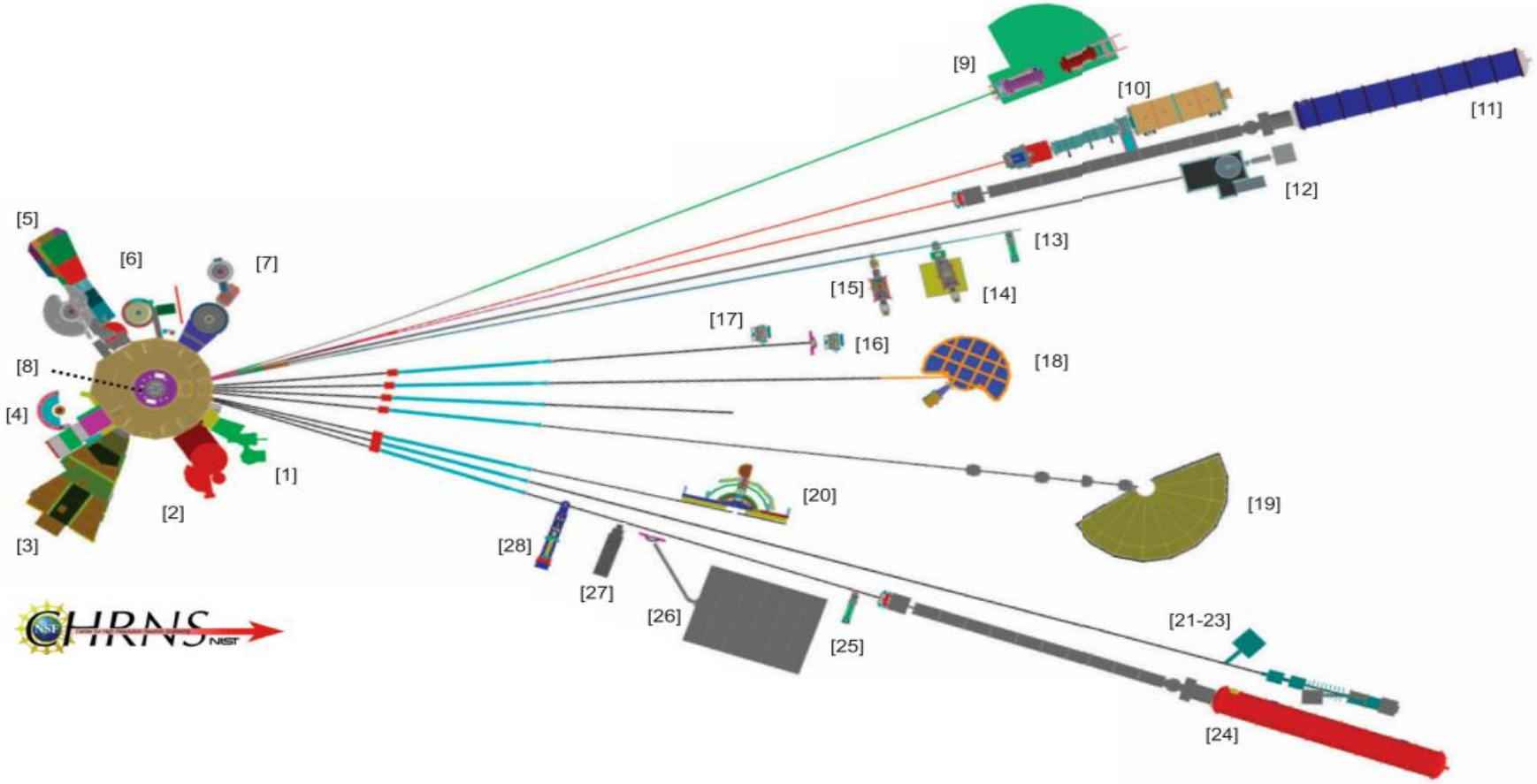
SPECTROSCOPY

STRUCTURE

SPECTROSCOPY: “interesting” portions of the sample are hydrogenated and the “uninteresting” portions are deuterated.

Neutron magnetic moment interacts with spins

Facility Layout

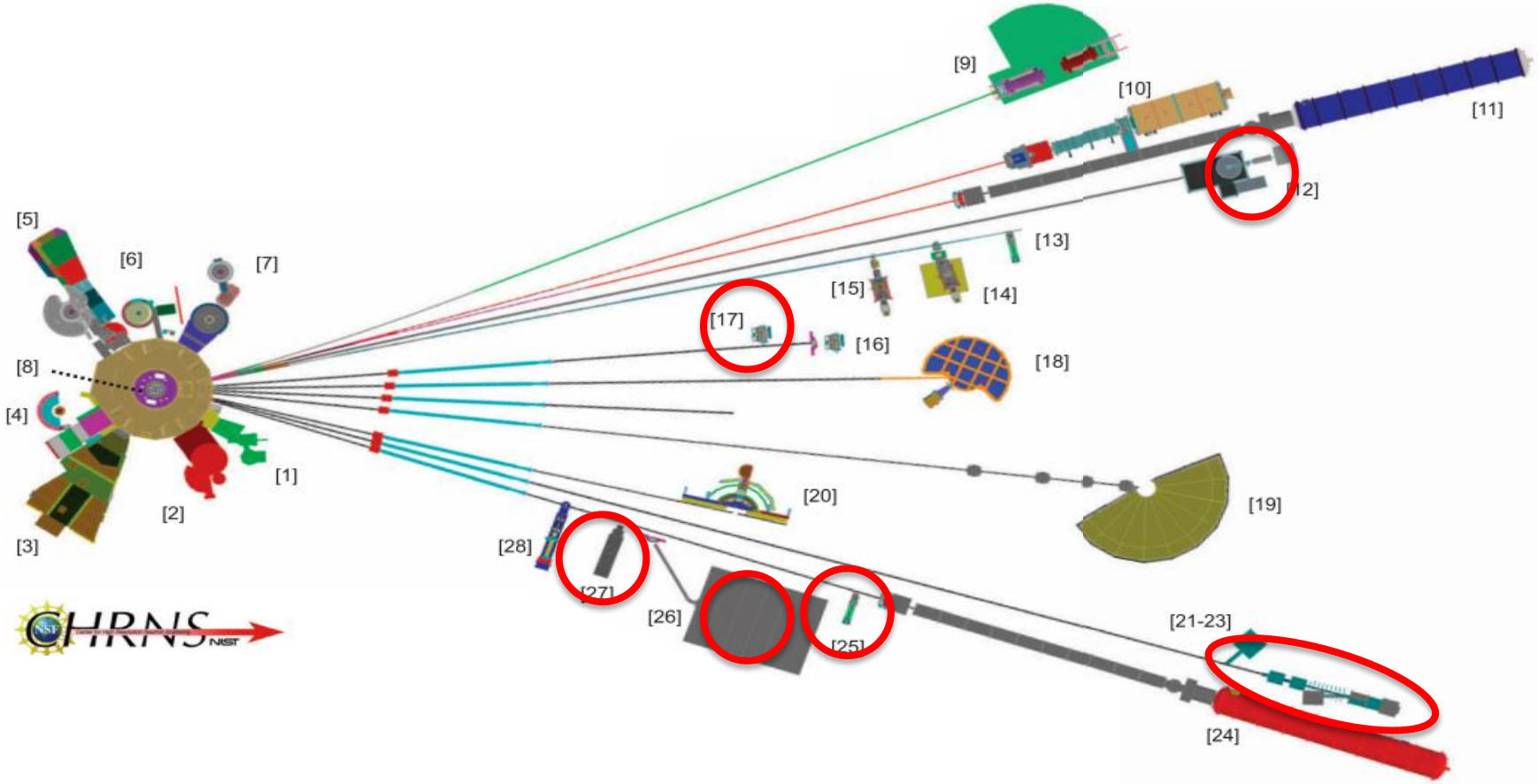


Facility Layout

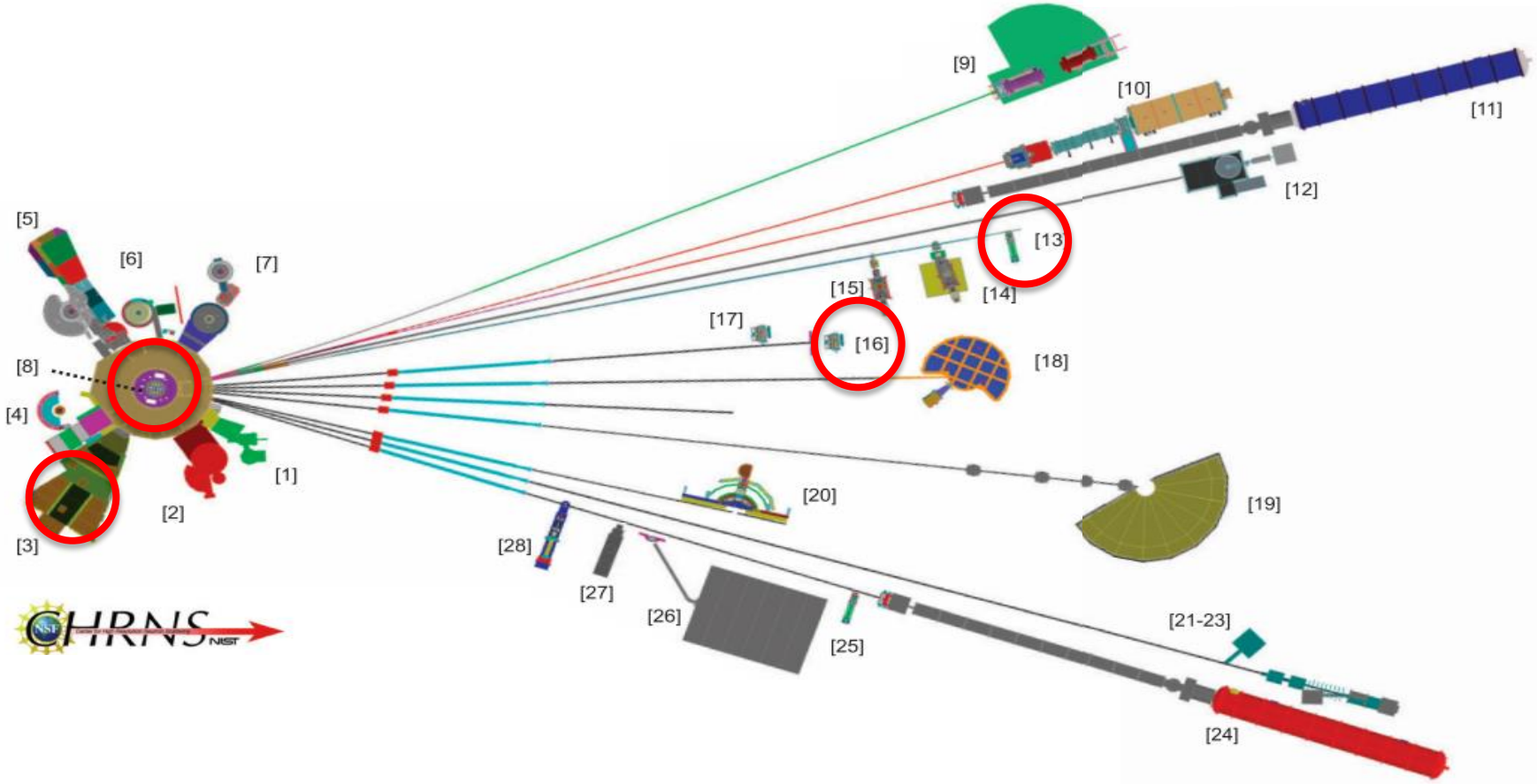
Facility Layout

Instrument Suites

Testing/Physics stuff



Absorption/Imaging



Absorption/Imaging

-Thermal Neutron Capture Prompt-Gamma Activation Analysis (PGAA)
-Cold Neutron Prompt-Gamma Activation Analysis (PGAA)

-Cold Neutron Depth Profiling (NDP)

-Neutron Imaging

Absorption/Imaging

-Thermal Neutron Capture Prompt-Gamma Activation Analysis (PGAA)
-Cold Neutron Prompt-Gamma Activation Analysis (PGAA)

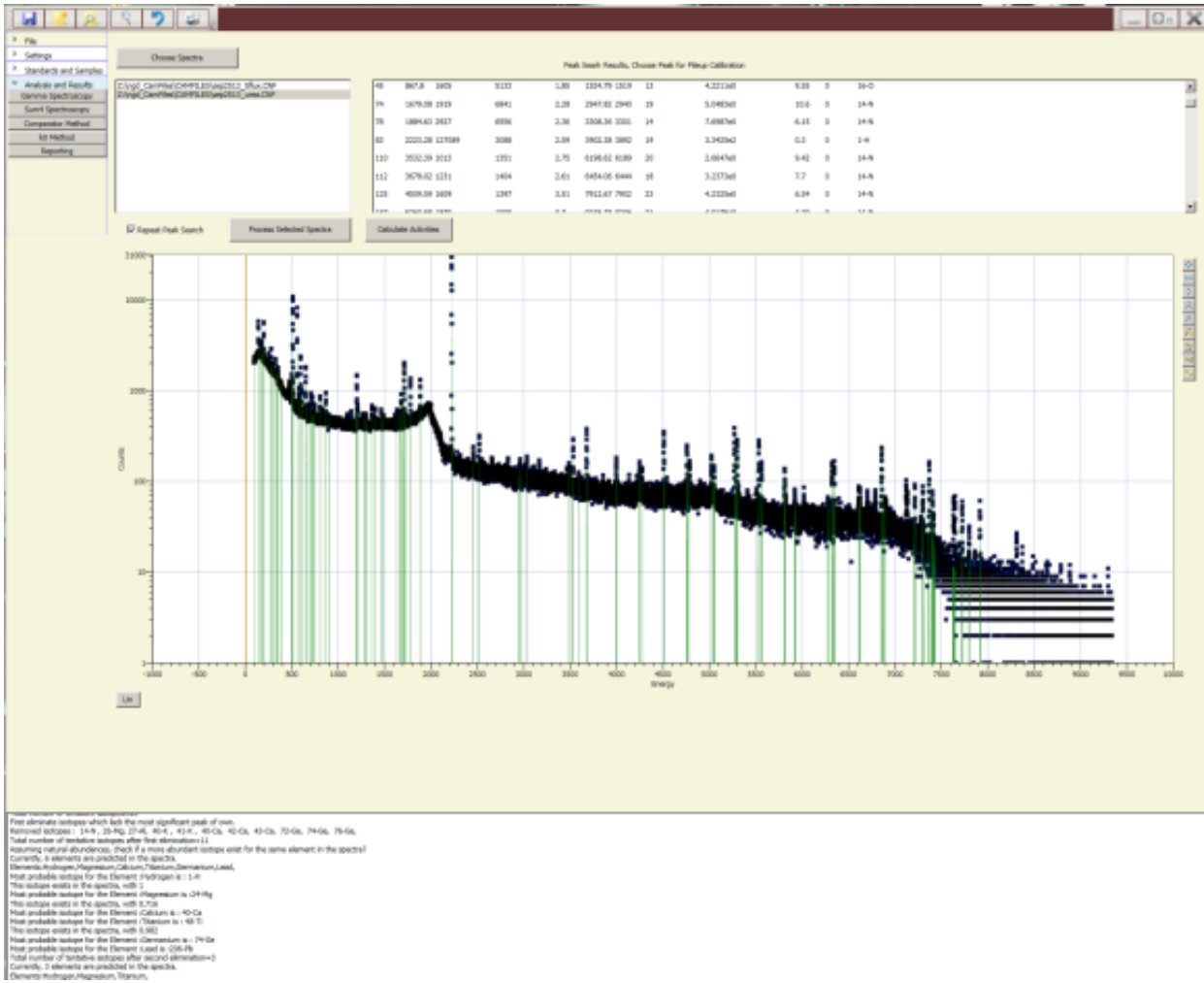
-Cold Neutron Depth Profiling (NDP)

-Neutron Imaging

Absorption/Imaging

Expected Sensitivity

Range (μg)	Elements
0.01 - 0.1	B, Cd, Sm, Gd
0.1 - 1	Eu, Hg
0.1 - 10	H, Cl, In, Nd
10 - 100	Na, S, K, Sc, Ti, V, Cr, Mn, Co, Ni, Cu, Ge, As, Se, Br, Mo, Ag, Te, I, Au
100 - 1,000	Mg, Al, Si, P, Ca, Fe, Zn, Ga, Rb, Sr, Y, Zr, Nb, Sb, Ba, La
1,000 - 10,000	C, N, F, Sn, Pb



Standard Reference Material 2387, $761

Standard Reference Material 3532, $711

Calcium-Containing Solid Oral Dosage
Dietary Supplement Health and Education Act (DSHEA)

Table 1. Certified Mass Fraction Values for Elements in SRM 3532

	Mass Fraction (mg/kg)			Coverage Factor, k
Cadmium (Cd)[a]	0.097 9	±	0.001 2	2.0
Calcium (Ca)[b,c]	175 200	±	3 300	2.0
Copper (Cu)[b,c,d]	280.7	±	7.6	2.0
Magnesium (Mg)[b,c]	11 800	±	200	2.0
Manganese (Mn)[b,c,d]	532	±	18	2.0
Zinc (Zn)[b,c]	2 110	±	40	2.0

Absorption/Imaging

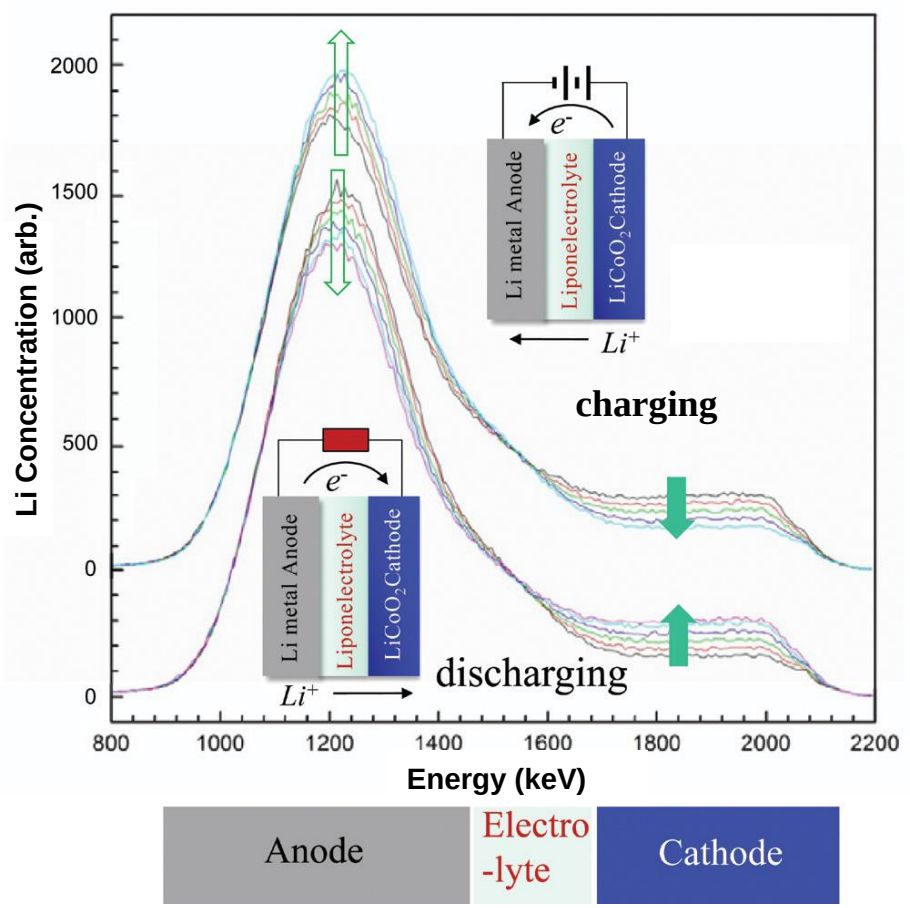
-Thermal Neutron Capture Prompt-Gamma Activation Analysis (PGAA)
-Cold Neutron Prompt-Gamma Activation Analysis (PGAA)

-Cold Neutron Depth Profiling (NDP)

-Neutron Imaging

Absorption/Imaging

- **B** in Semiconductors - various
- **Li** in Nuclear Waste Glasses
- **N** in Specialty Glasses & Metal CRMs
- **Li** in Lithium Ion Batteries
- **Na** in Steel Coupons
- **O** in Titanium oxides



* Data and images courtesy of Greg Downing

Absorption/Imaging

- **B** in Semiconductors - various
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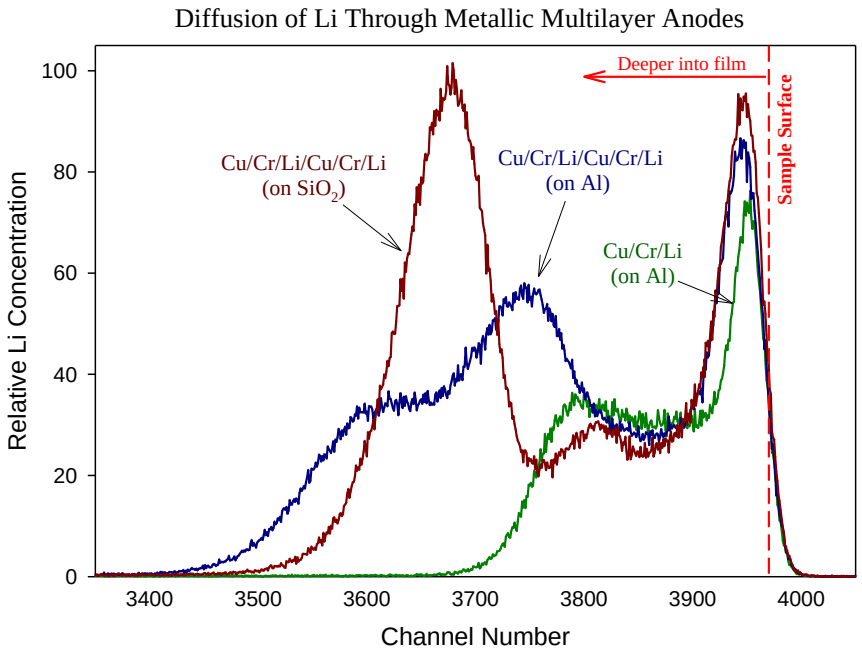

* Data and images courtesy of Greg Downing

Absorption/Imaging

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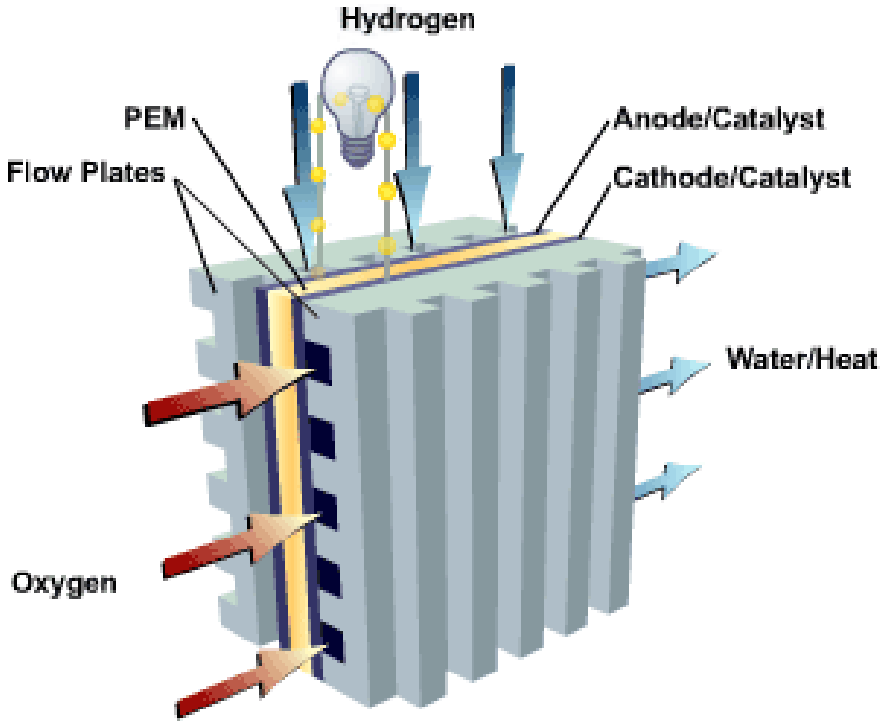
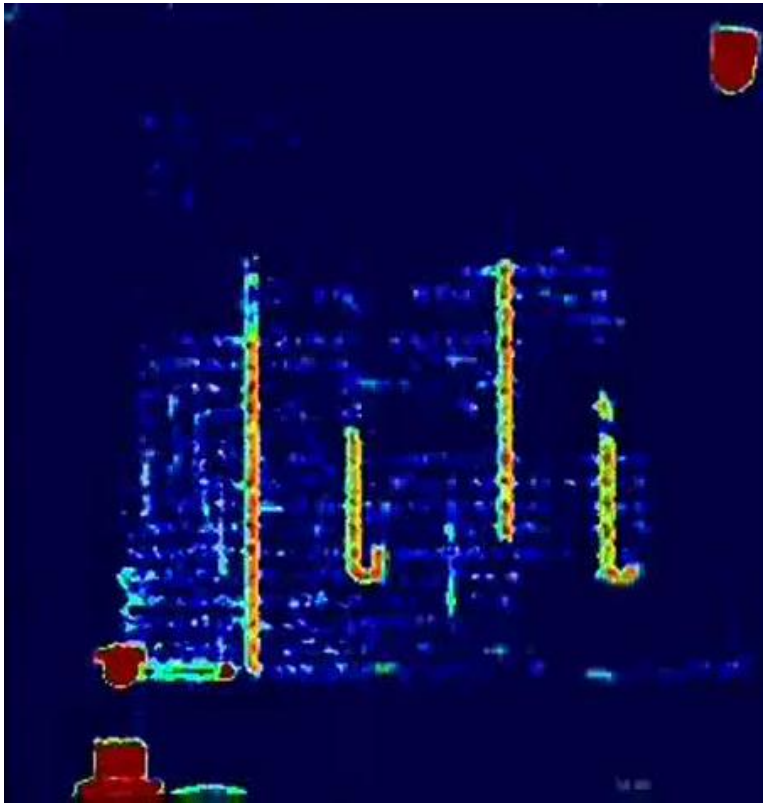
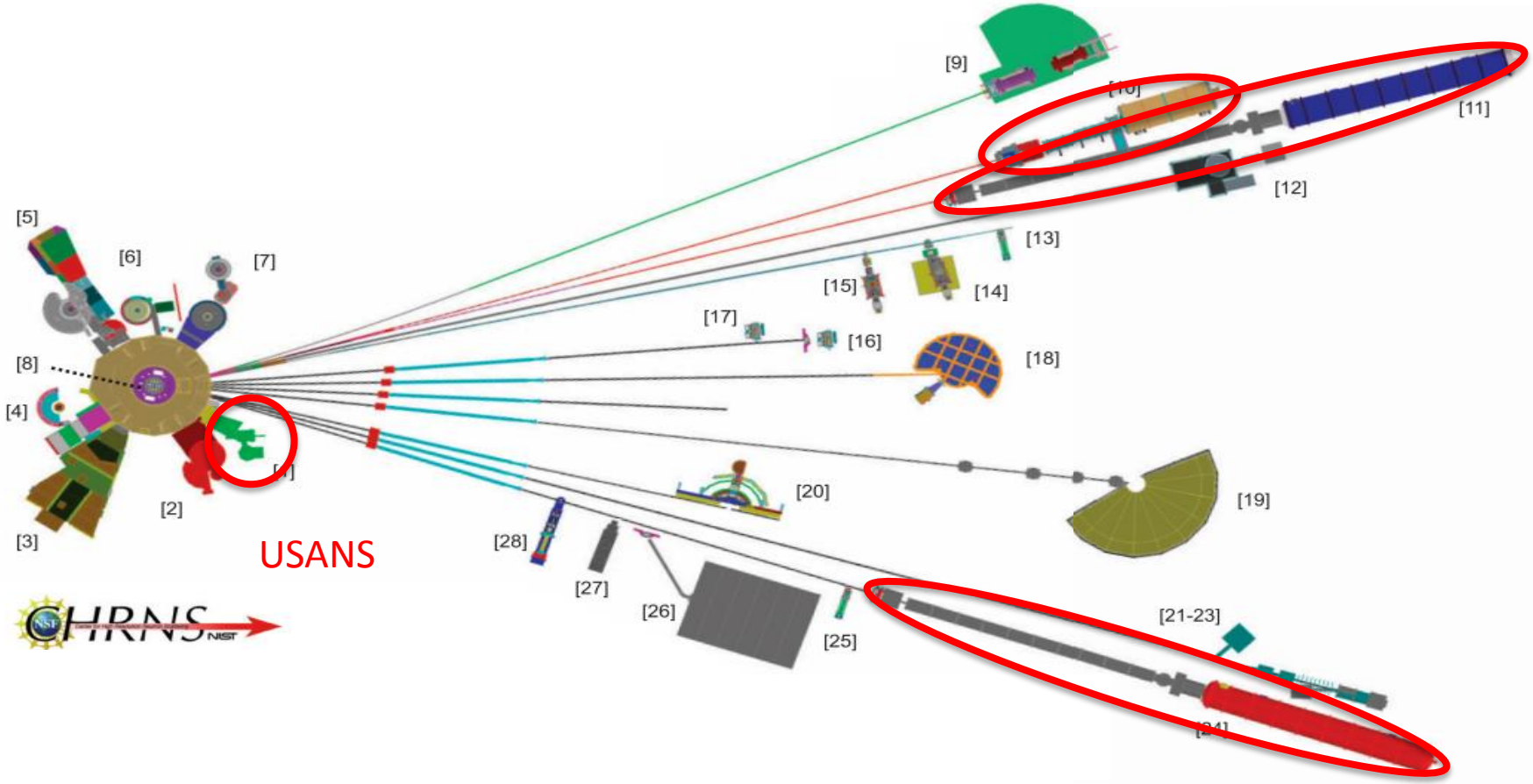


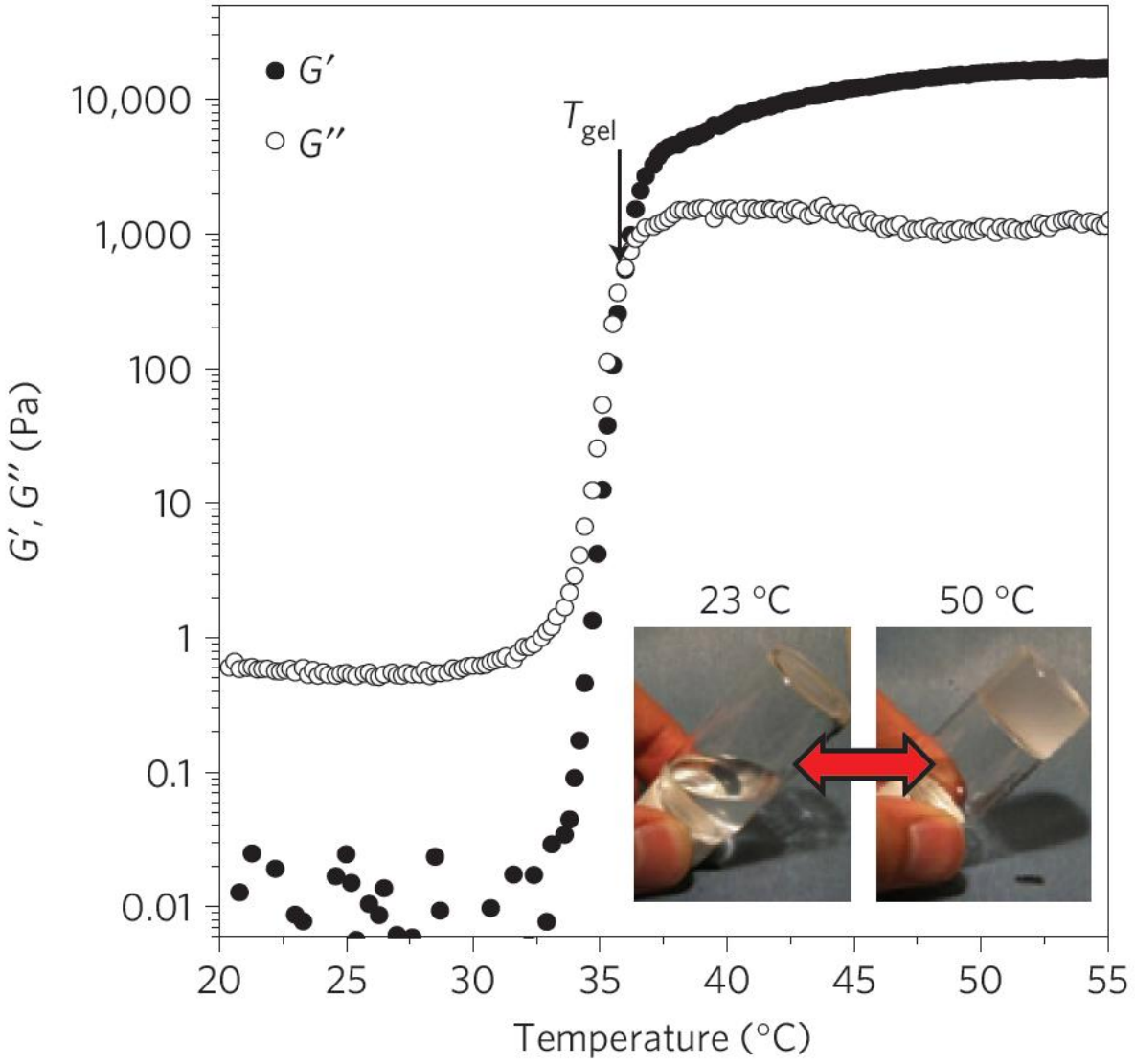


* Data and images courtesy of David Jacobson

Small-Angle Neutron Scatt….(SANS)



Mesoporous Organohydrogels



oil-in-water nanoemulsions

=> silicone oil (PDMS) droplets
[polydimethylsiloxane, (PDMS)]

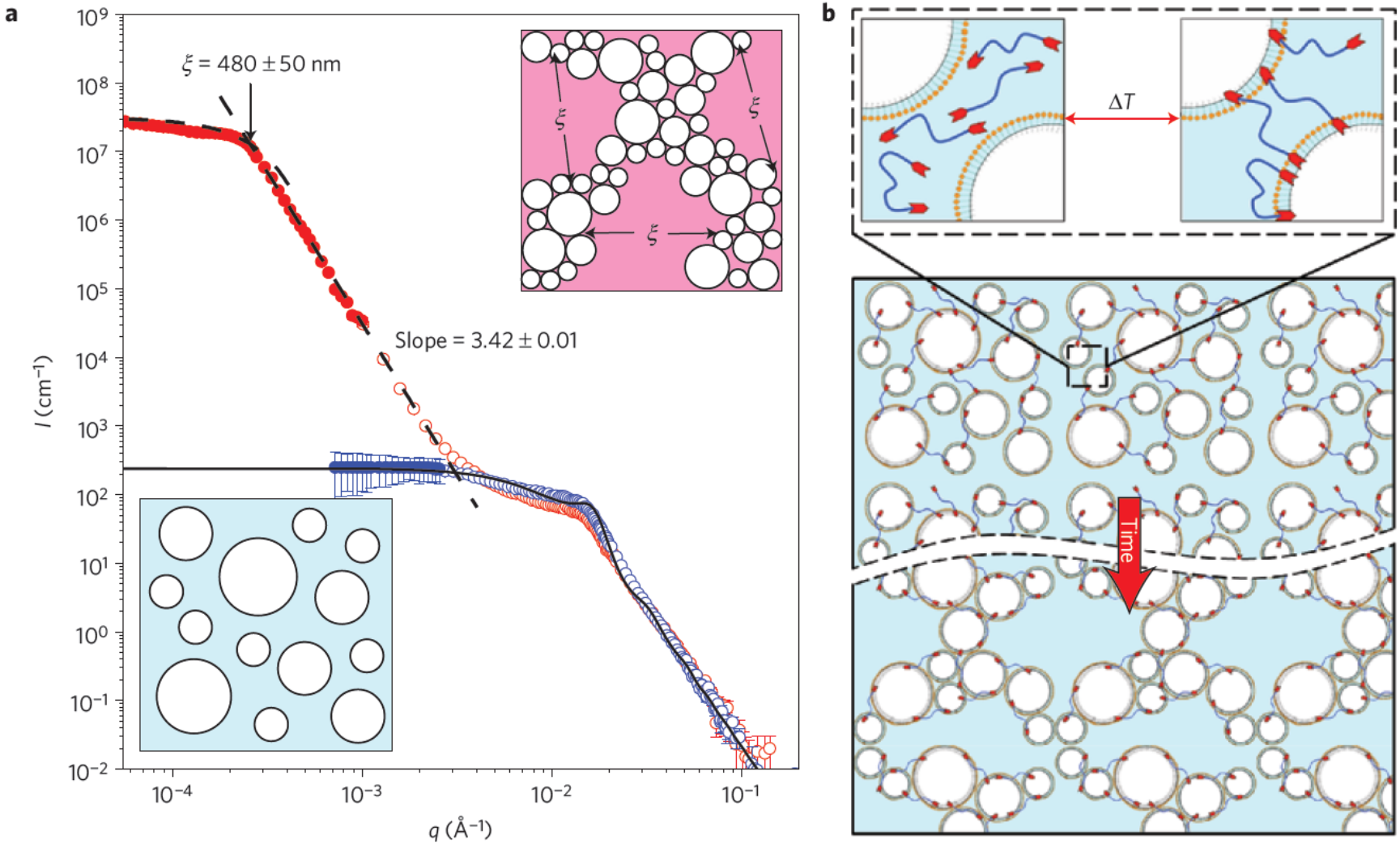
=> aqueous continuous phase
[18% D_2O]

=> functionalized hydrophilic polymer
[poly(ethylene glycol) diacrylate (PEGDA)]

=> surfactant (SDS)

* Data and images courtesy Paul Butler et al.

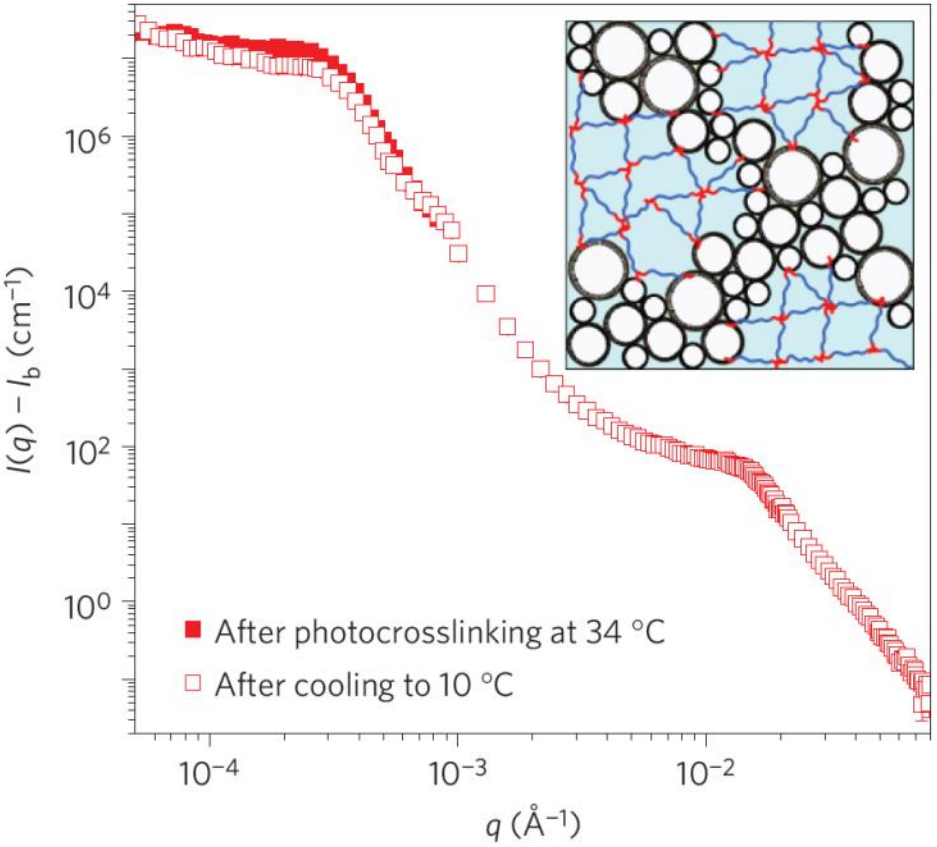
Mesoporous Organohydrogels

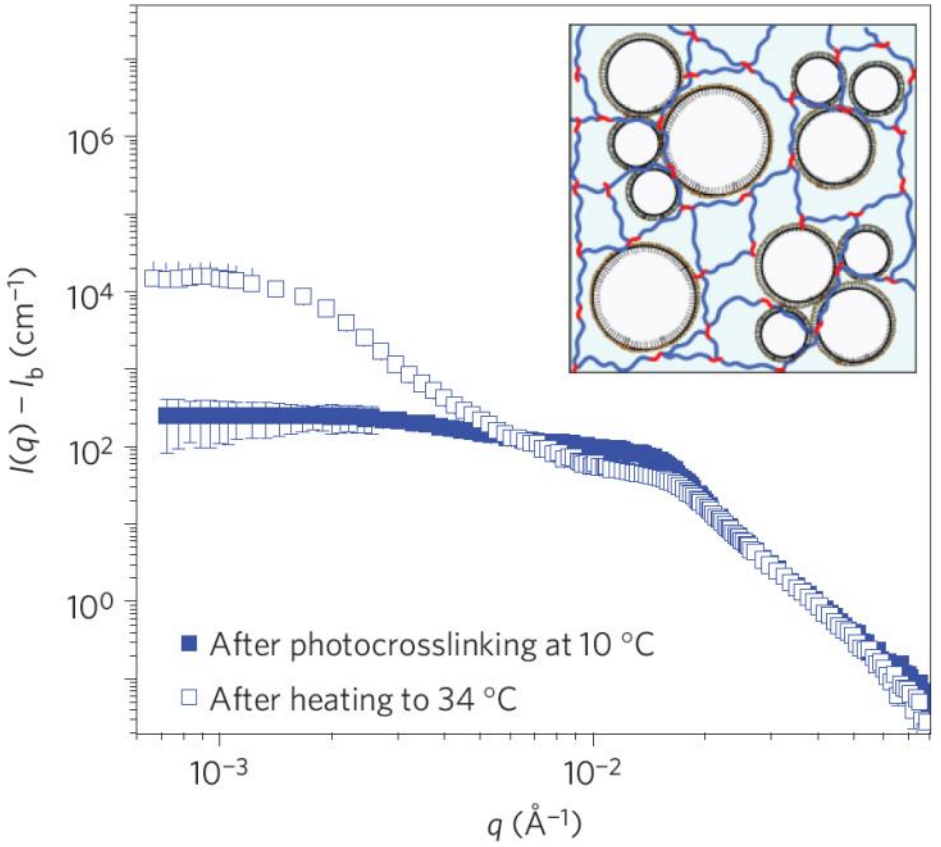


M.A. Helgeson, *et al.,* Nature Materials **11**, 344 (2012)

Mesoporous Organohydrogels

After Photocrosslinking





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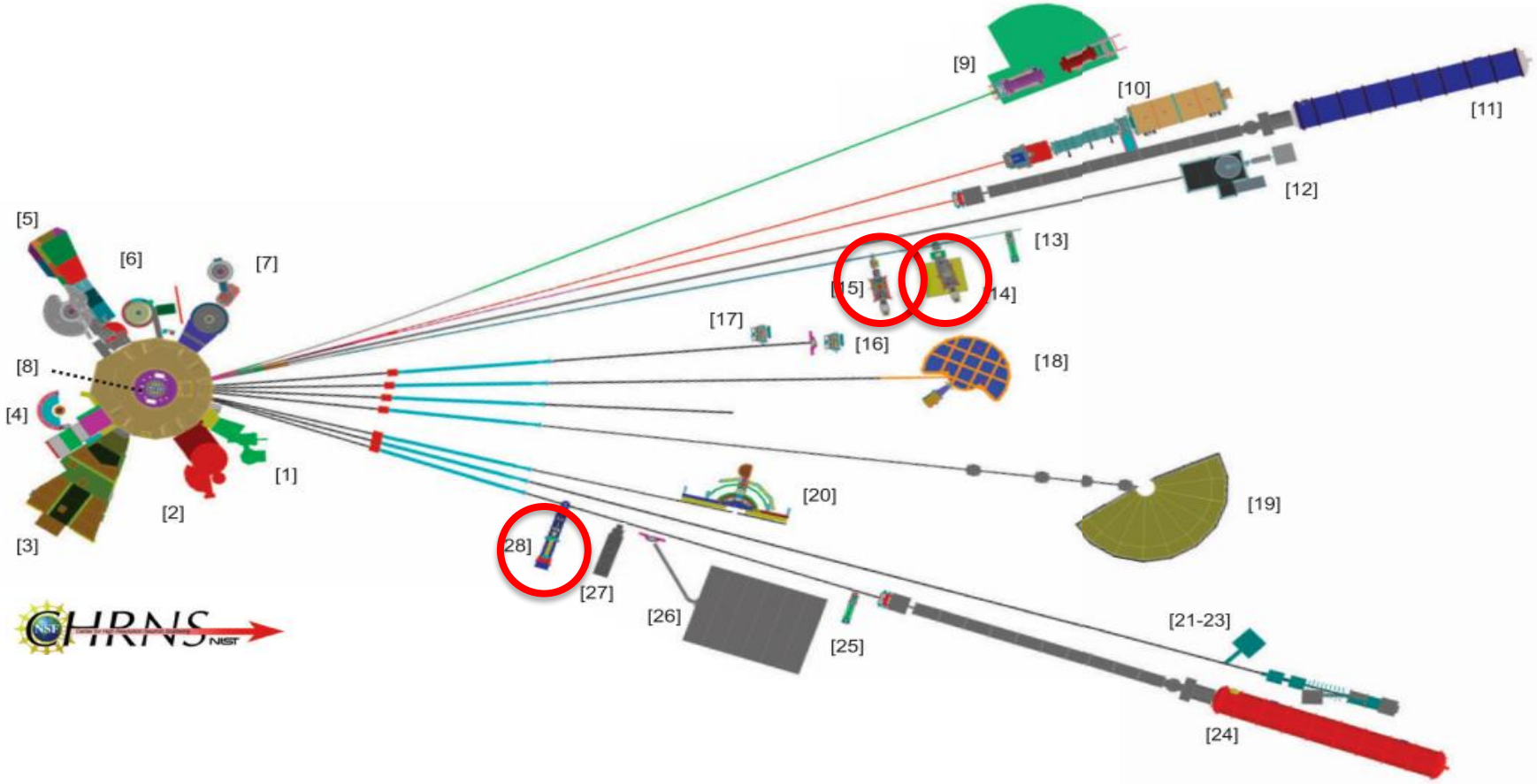
Reflectometers



Reflectometers

- NG-7 Horizontal Sample Reflectometer allows reflectivity measurements of free surfaces, liquid/vapor interfaces, as well as polymer coatings.

- NG-D Polarized Beam Reflectometer (PBR) for measuring reflectivities as low as 10^{-8} to determine subsurface structure

- NG-D MAGIK off-specular reflectometer for studies of thin-film samples with in-plane structure.

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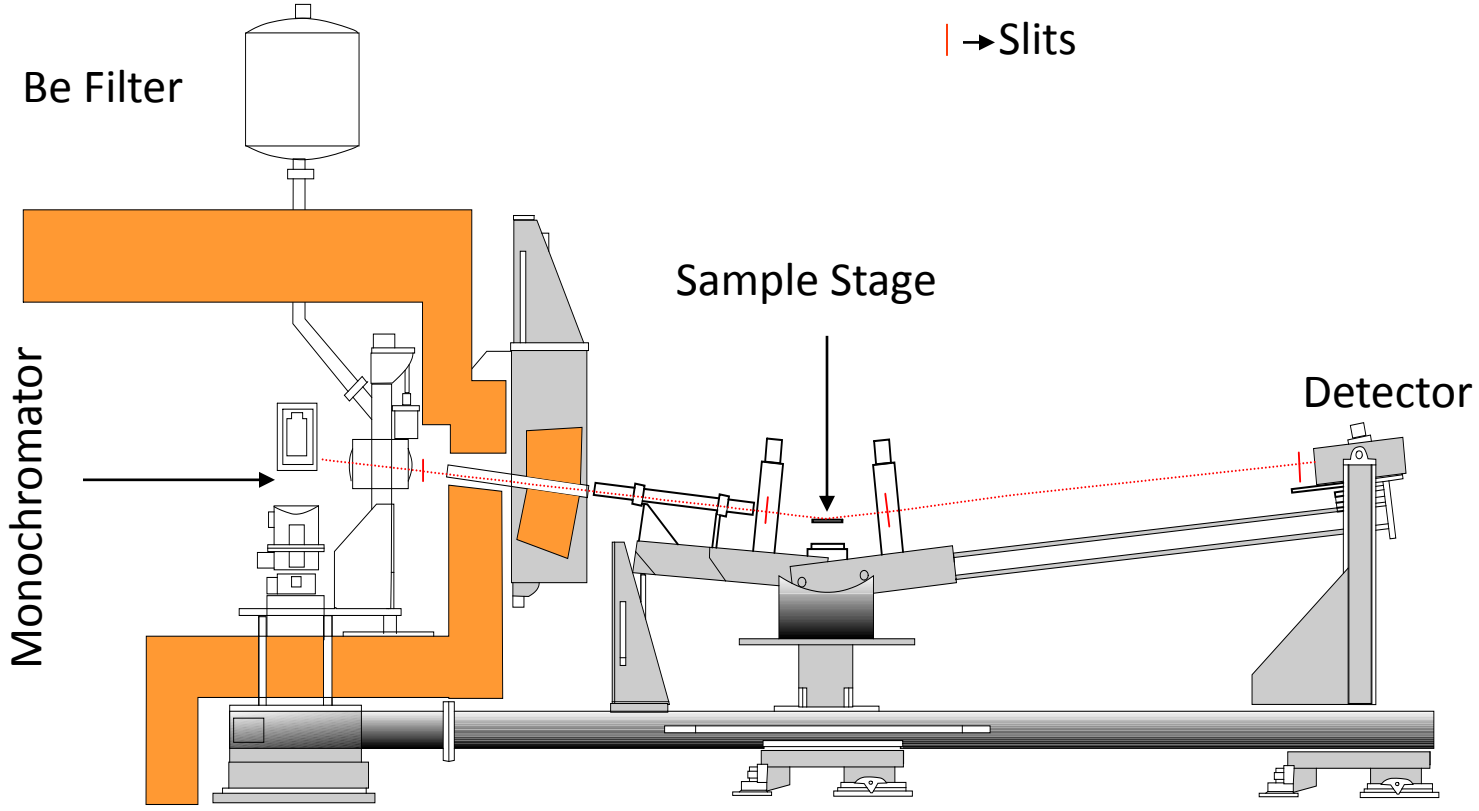


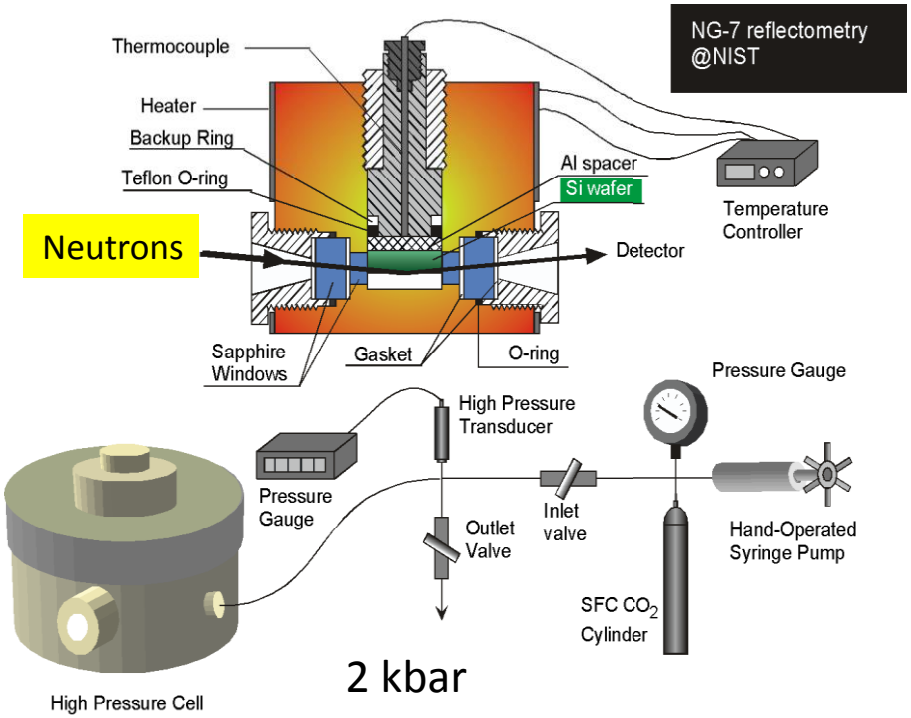
* Data and images courtesy Sushil Satija

Reflectometers

Replace organic toxic solvents by CO_2 as a "green" solvent for polymer processing.
(~74 bar @ room temperature)

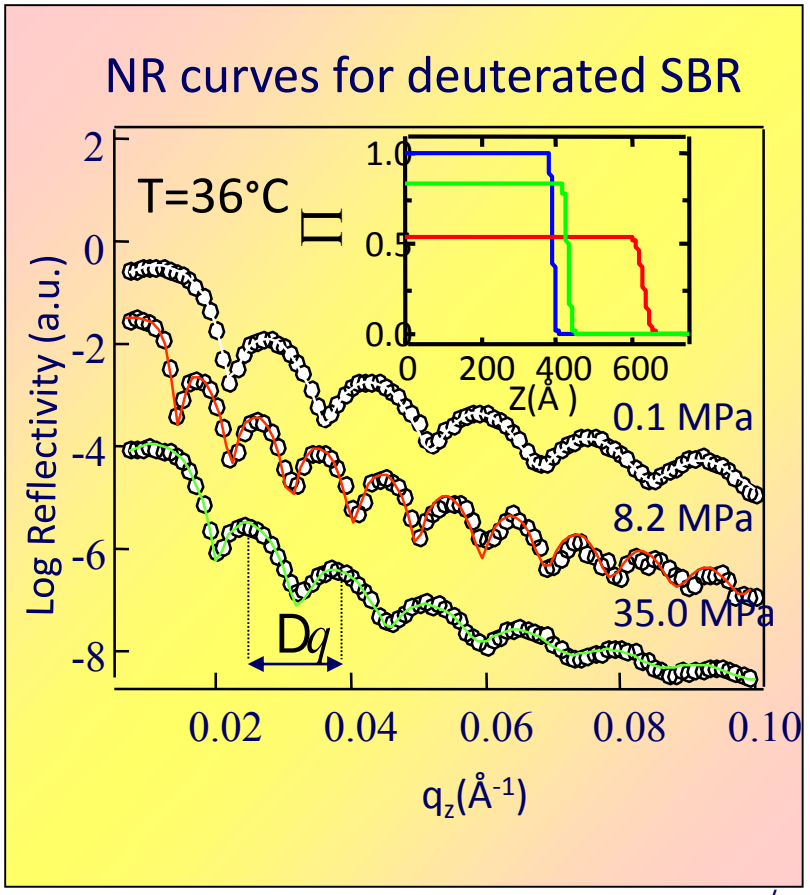
Supercritical fluid: anomalous behavior in sound velocity, thermal conductivity, partial molar volume.

Schematic view of high pressure cell for NR experiments



(Koga et al. *Macromolecules*, 2003)

NR curves for deuterated SBR



$D = 2p/Dq$

D: film thickness

$q_z = 4\pi \sin\vartheta/\lambda$

λ : wavelengt

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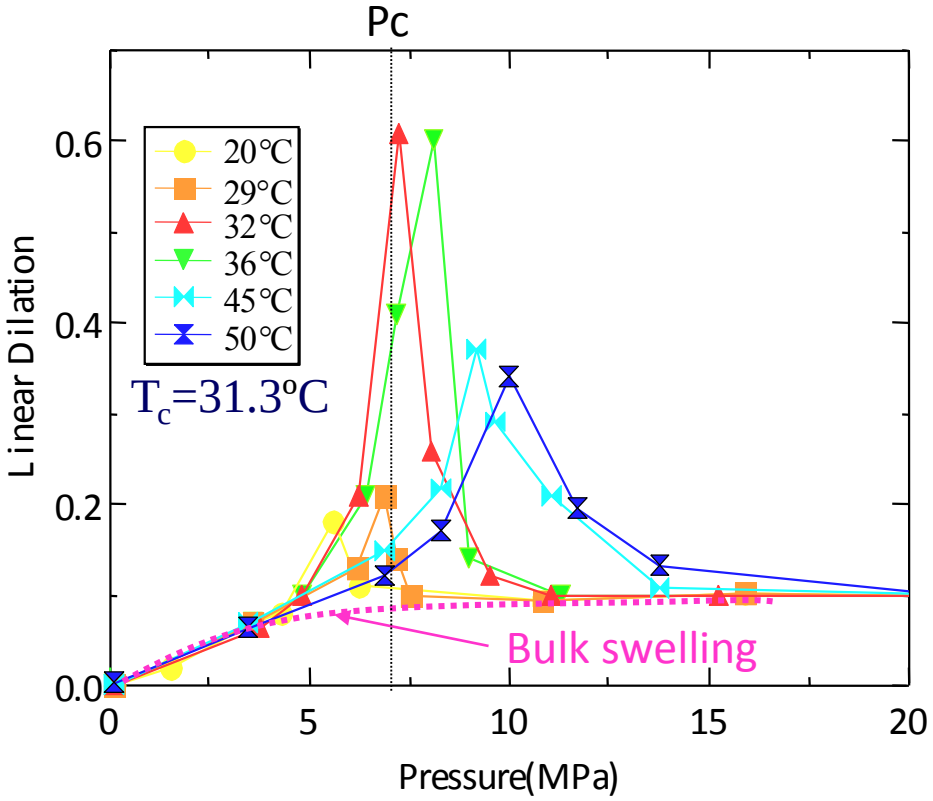

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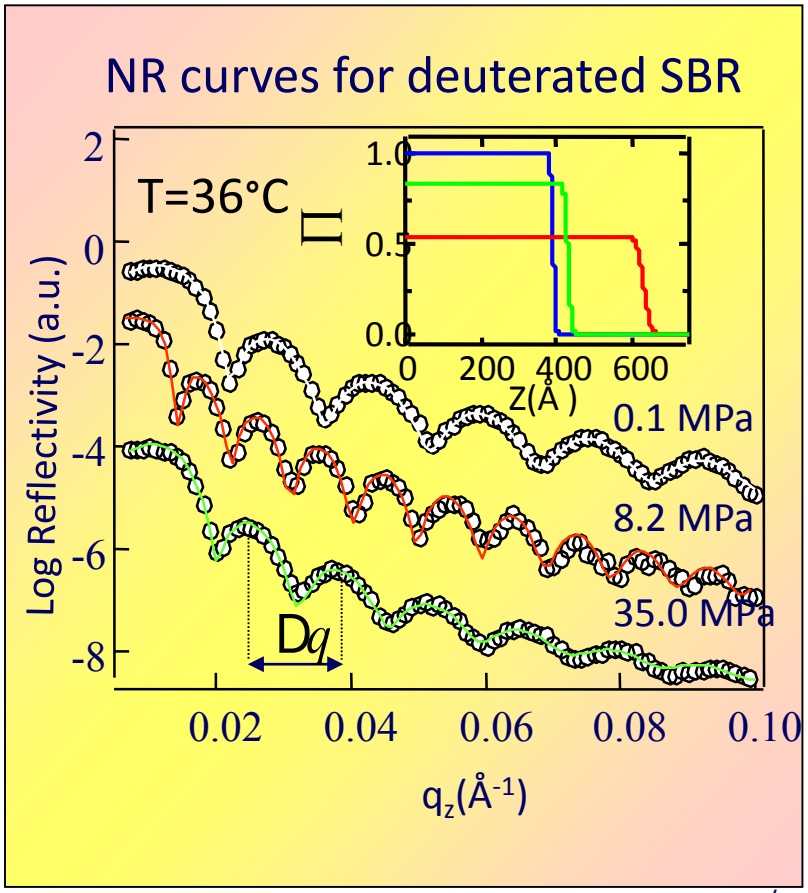

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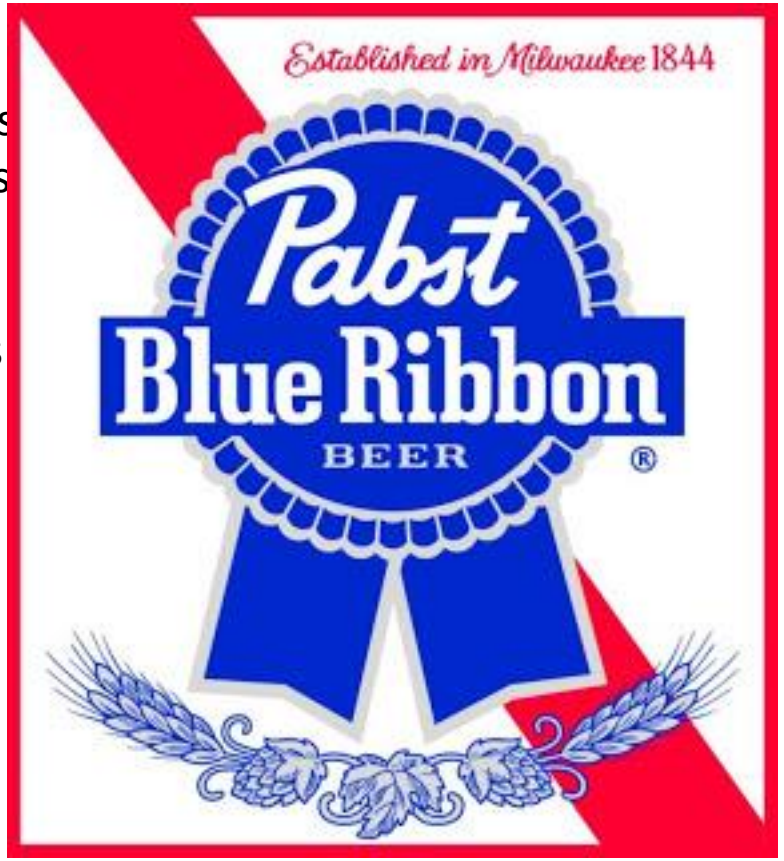
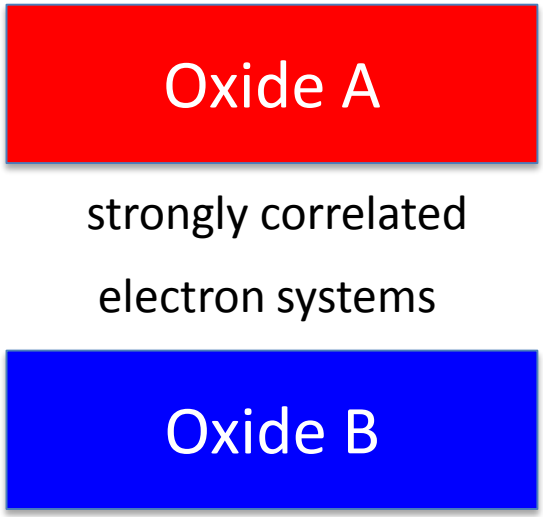
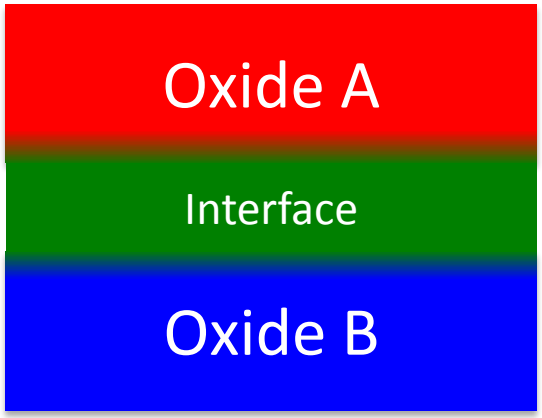


Reflectometers

complex oxide interfaces





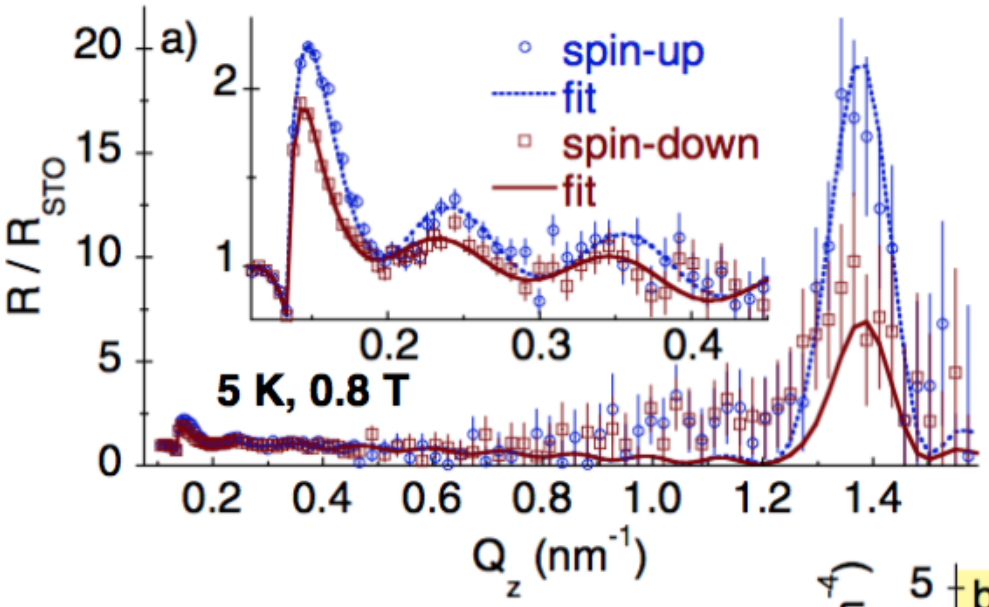
due to strain, charge transfer, etc.,
new properties can emerge at the

interface between A & B!

ferromagnetism, superconductivity, ...

$[CaMnO_3 / CaRuO_3]_N$

antiferromagnetic insulator ***paramagnetic metal***

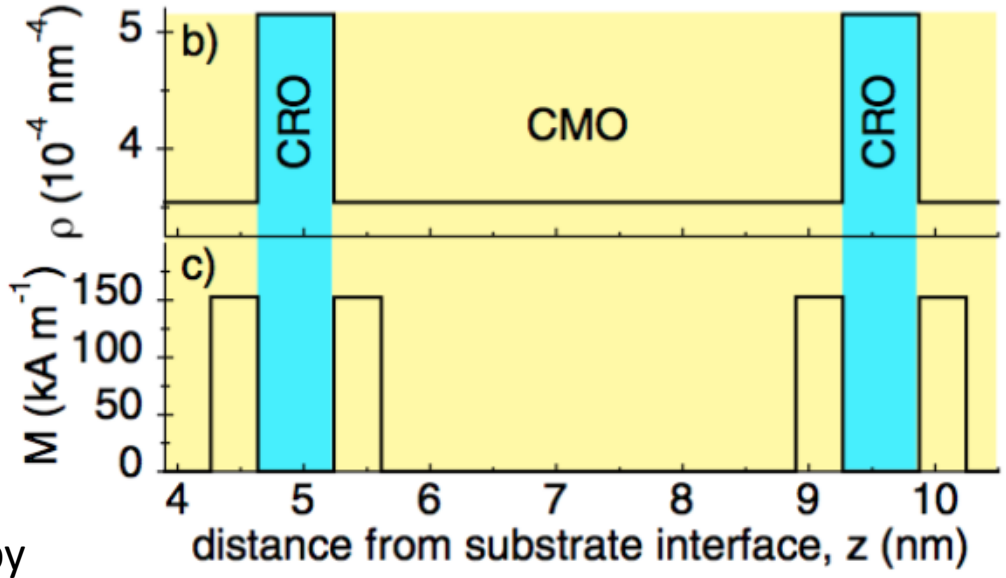


spin-dependent oscillations & 1st order Bragg peak

small samples limit *Q*-range

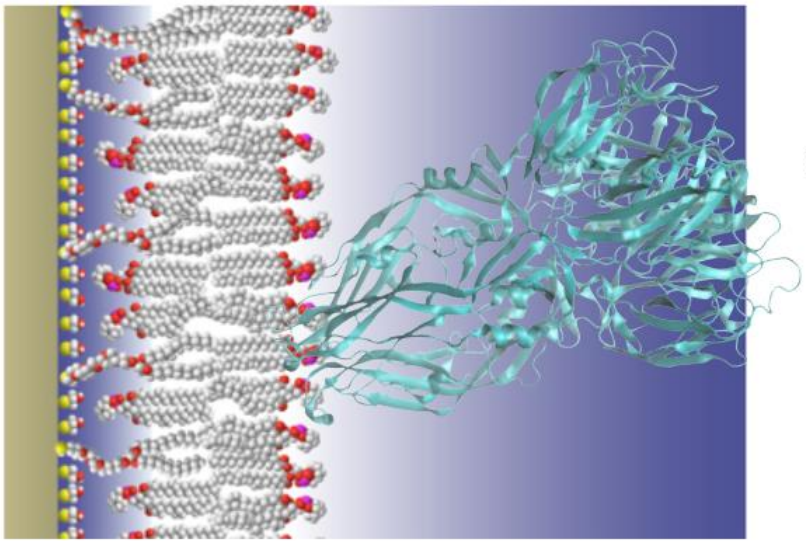
consistent with 1 unit cell interfacial ferromagnetism

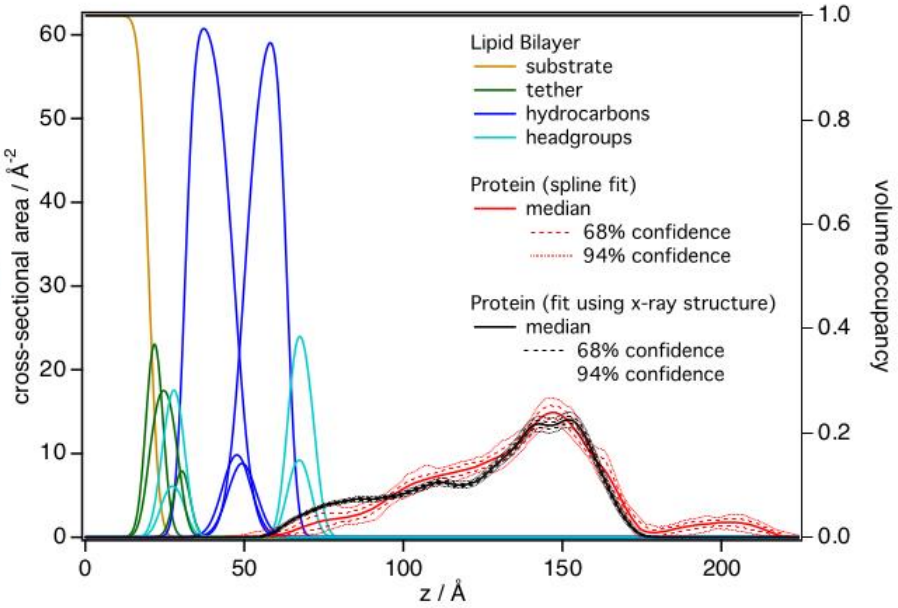
controllable with E-field



* Data and images courtesy of Brian Kirby

Dengue envelope protein



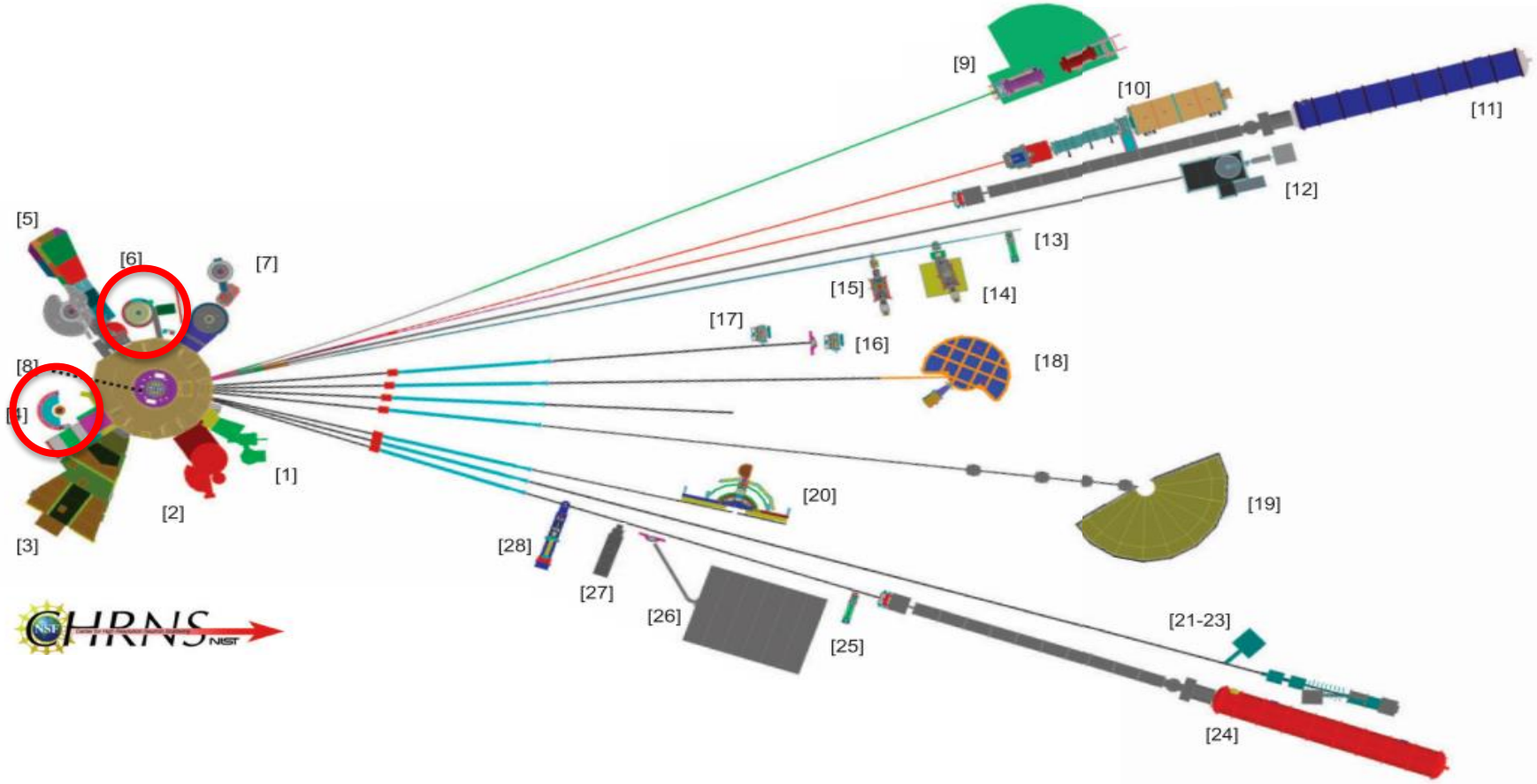


- in collaboration with Mike Kent, Bulent Akgun, Sandia National Laboratories
- main objective: insertion depth of the protein into the bilayer

* Data and images courtesy of Frank Heinrich

manuscript in preparation

Diffractometers



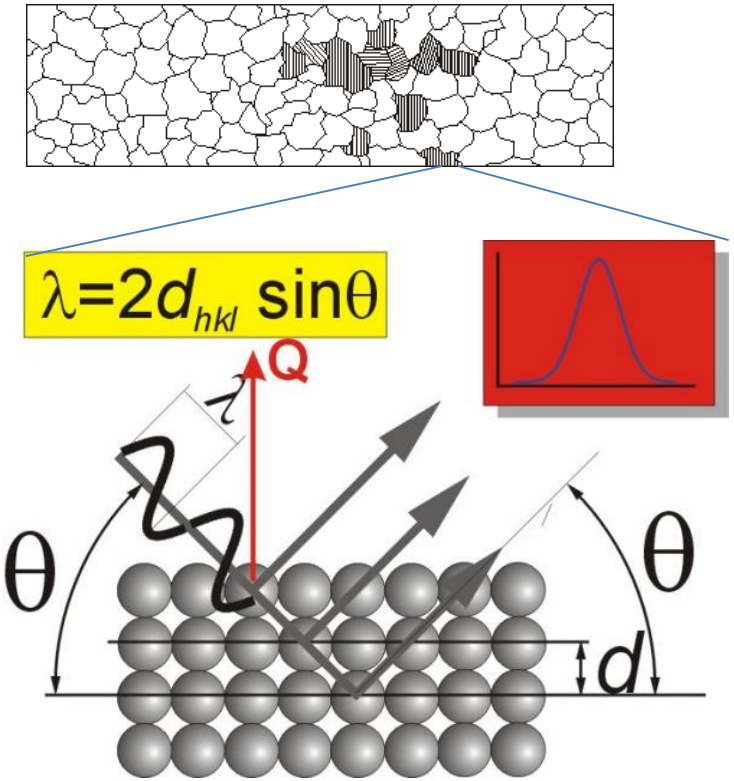
Diffractometers

- BT-8 Stress-strain engineering diffractometer

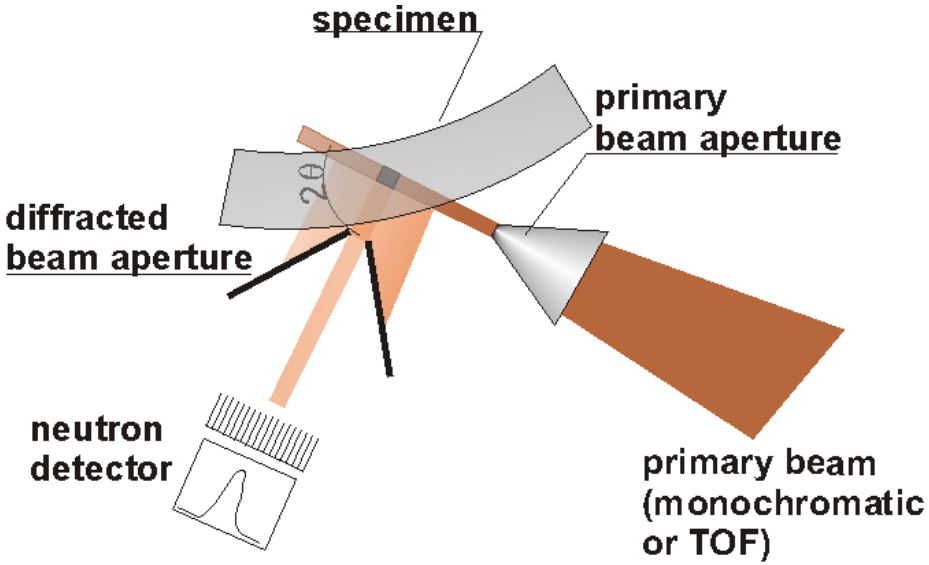
- BT-1 High resolution powder diffractometer

Neutron Stress Measurements

Elastic changes of lattice spacings in grains provide strain information



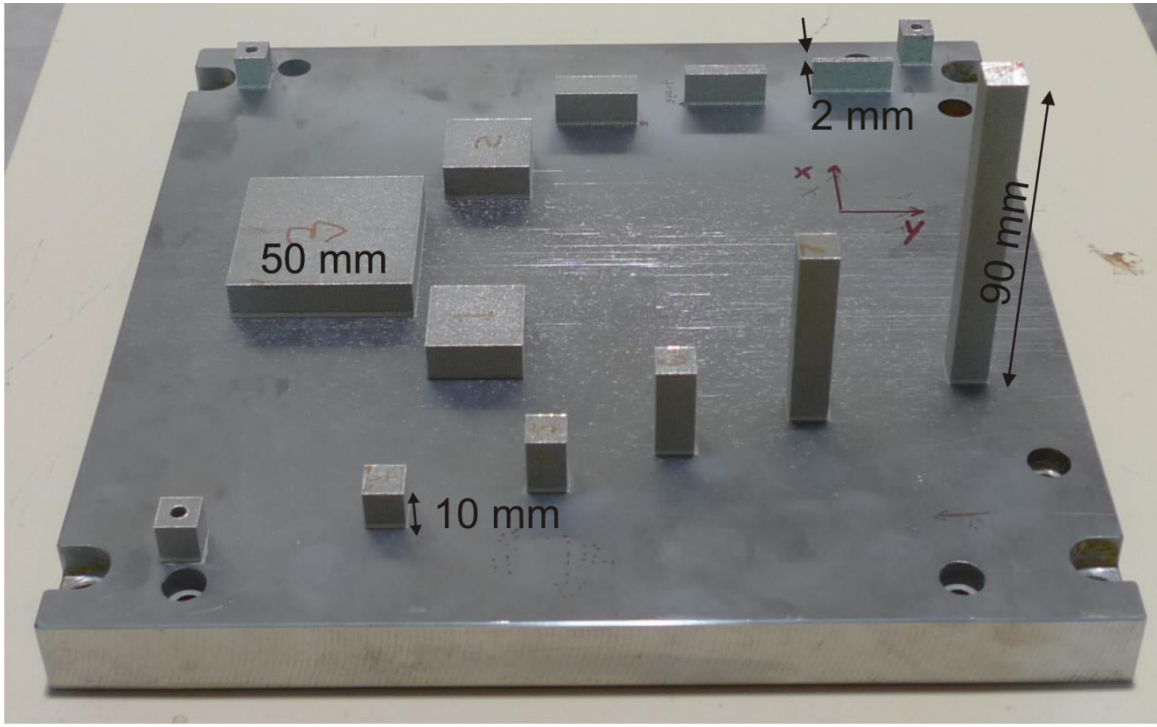
Penetration of neutrons (≈ cm) provides non-destructive depth information



* Data and images courtesy of Thomas Gnäupel-Herold

Sample and Equipment

- **EOSINT M 280 laser sintering machine (400 watt Yb laser, 0.1..0.5 mm focus, 7 m/s scan speed**
- **GP1 powder (15.5% Cr, 4.5% Ni, 3.5% Cu, 0.4%Mn, 0.3% Nb, 0.5% Si, Fe bal.), is equivalent to 17-4 stainless steel,**
- **17-4: $Y_{min} \approx 724…1172$ MPa (depends on heat treatment)**



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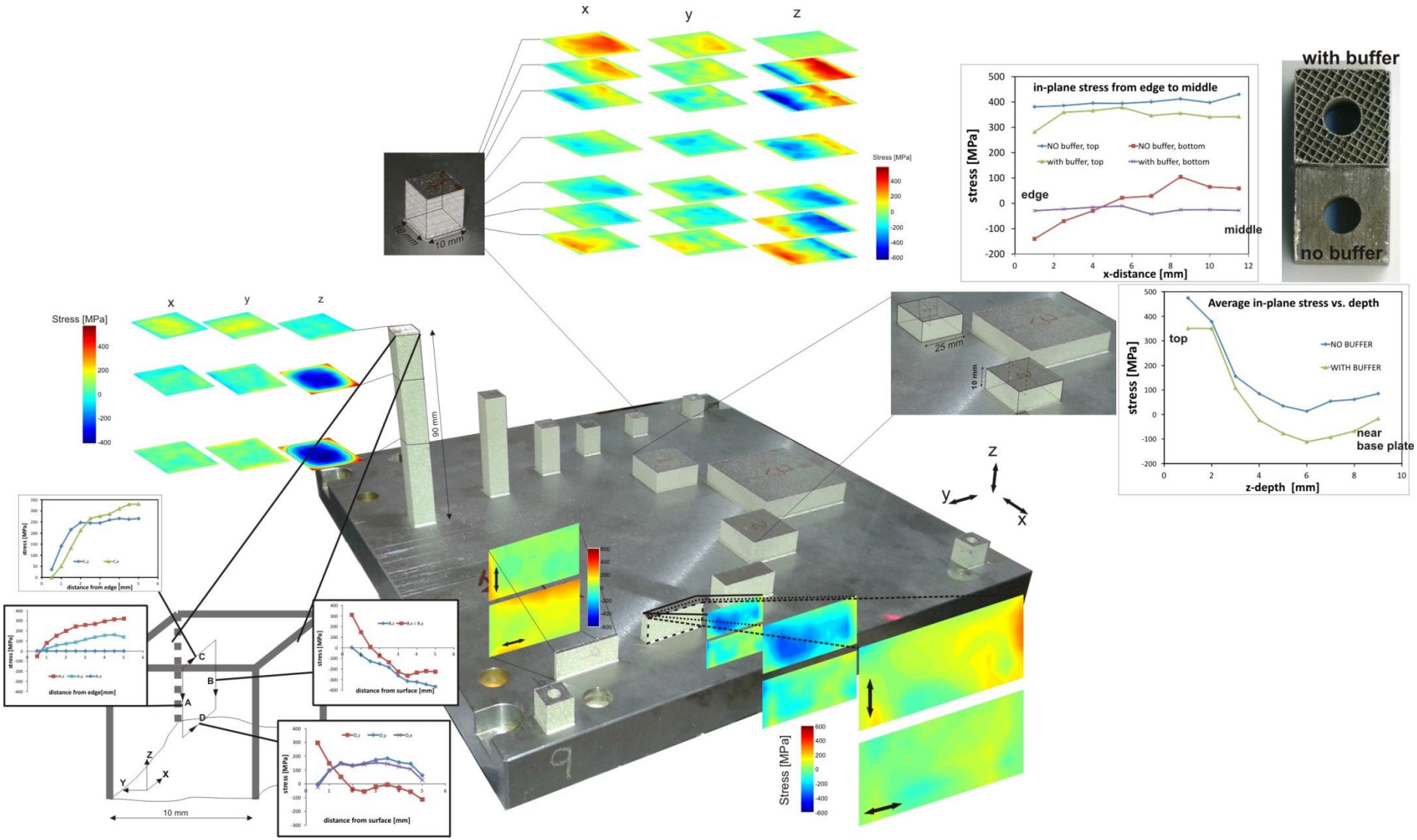
Stresses



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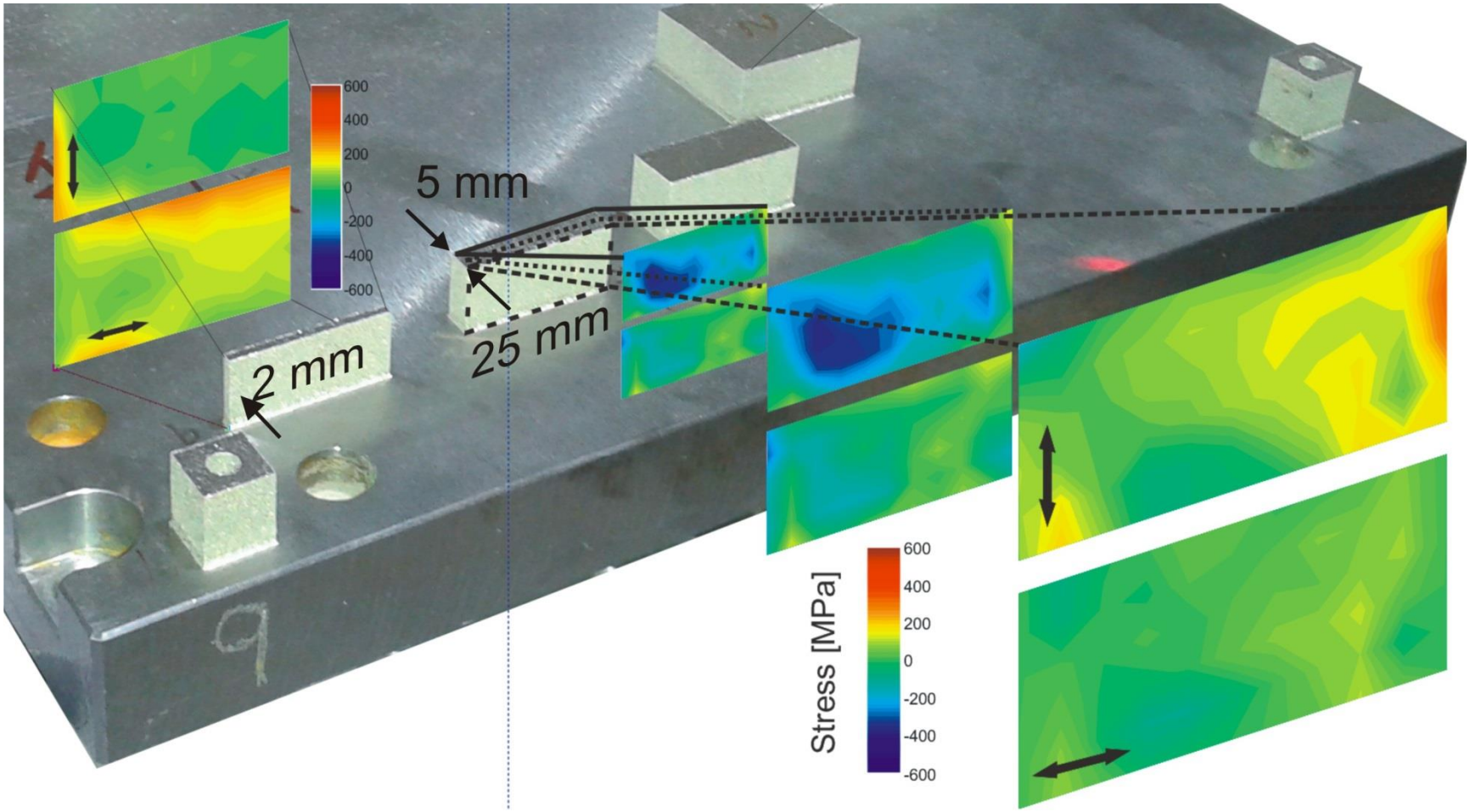
Stresses in “blade” structures



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Diffractometers

- BT-1 High resolution powder diffractometer

- BT-8 Stress-strain engineering diffractometer

Industrial gas separations

Other Chemical Separations
i.e. Natural Gas

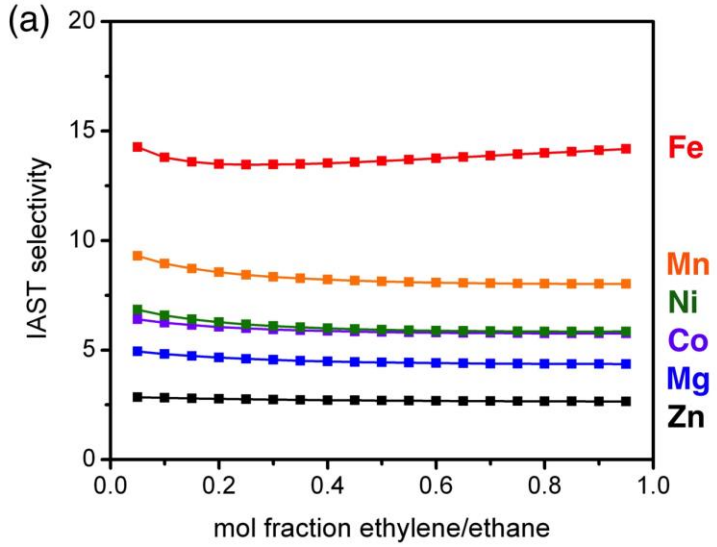
Contains
CH_4
C_2H_6
C_3H_8
C_4H_{10}
etc….

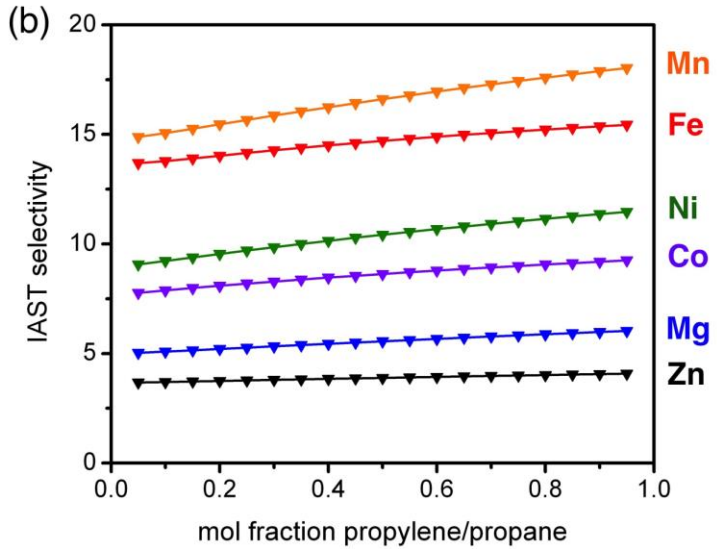
$H_2/CH_4/CO/CO_2$

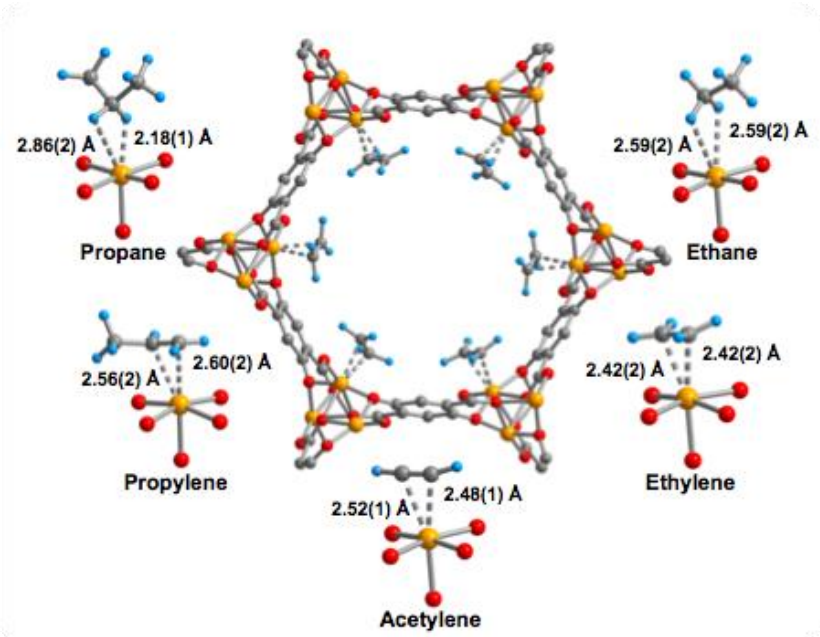
O_2/N_2

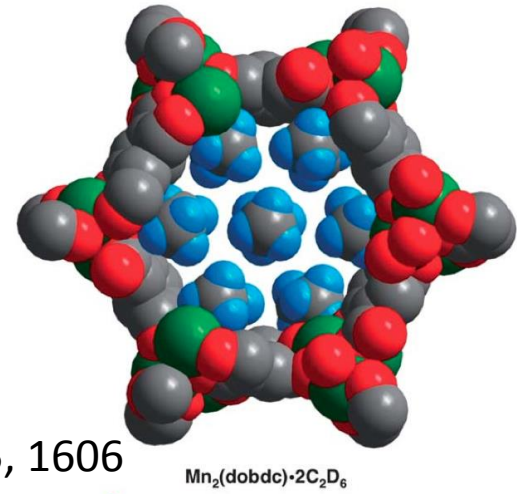
Olefin/paraffin

Diffractometers



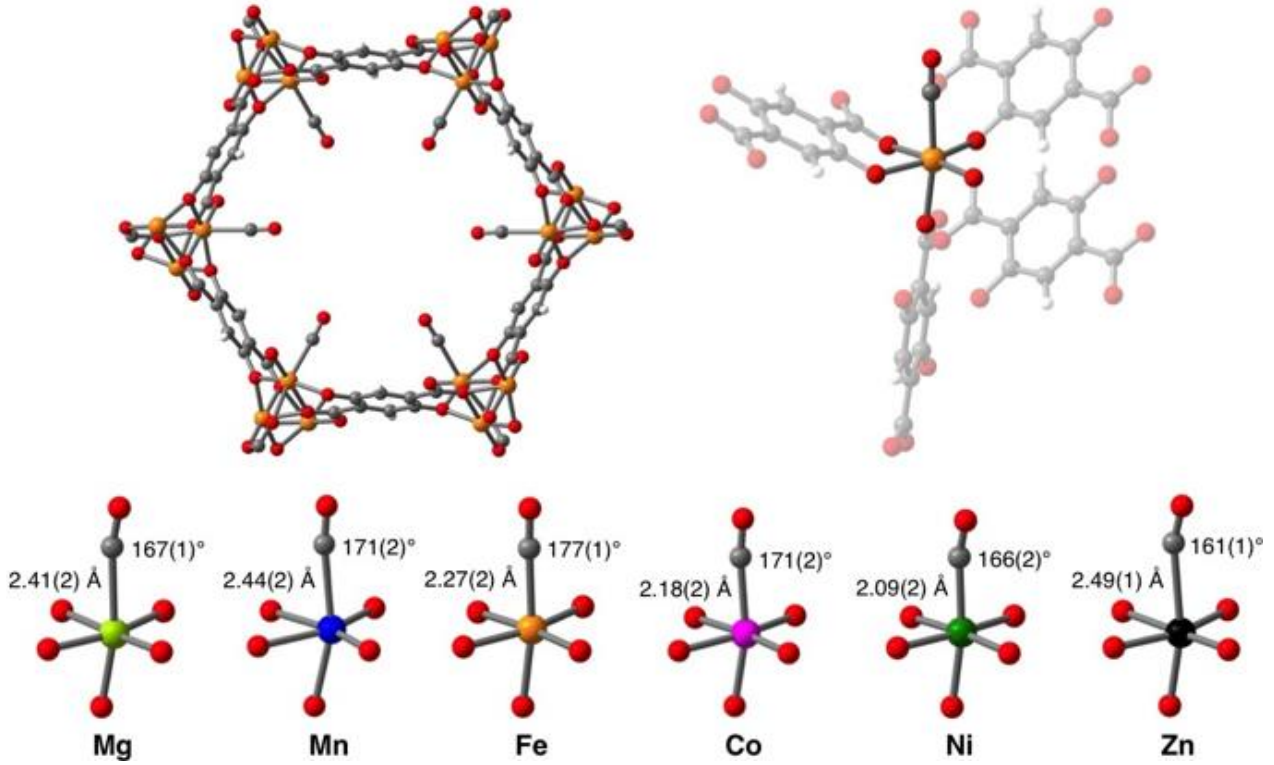






Bloch et al., Science 2012, 335, 1606

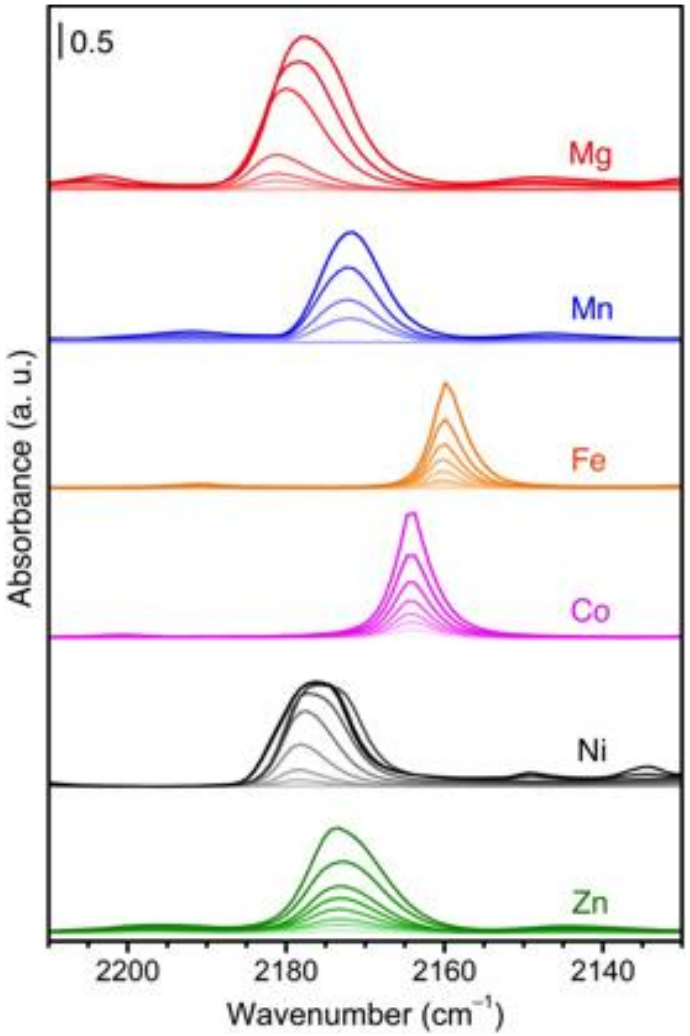
Diffractometers

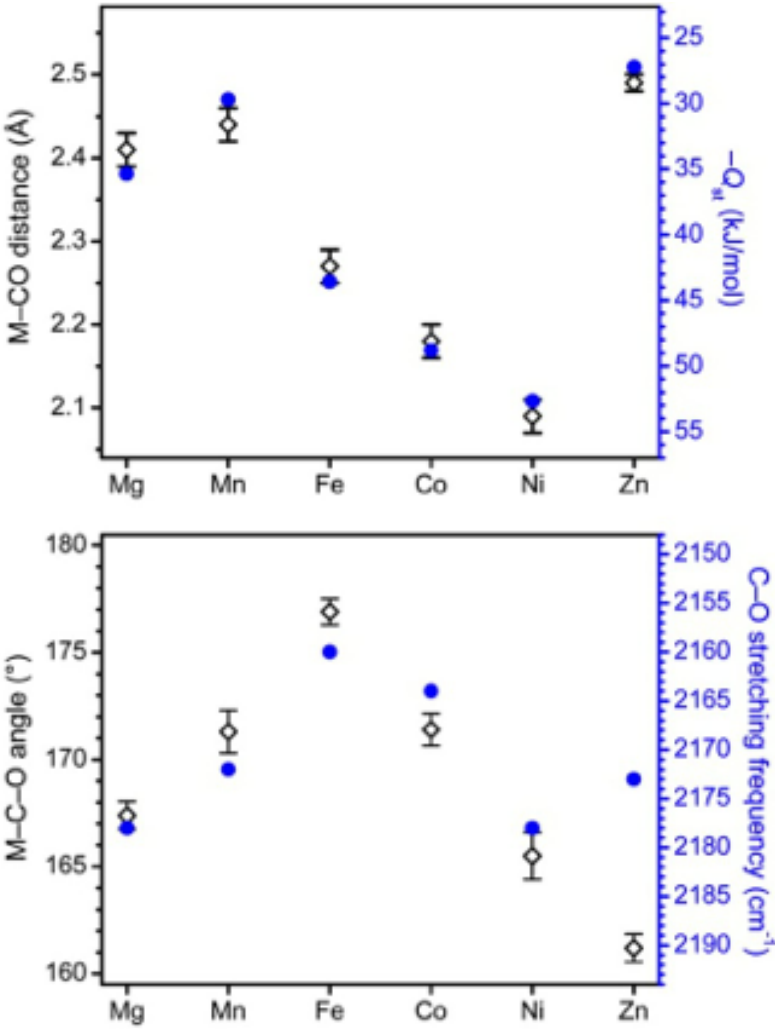


The first crystallographically characterized magnesium and zinc carbonyl compounds
The first high-spin manganese(II), iron(II), cobalt(II), and nickel(II) carbonyl species

Bloch et al., J. Am. Chem. Soc. 2014
JACS Spotlight “Molecular Boxes Act like Little Carbon Monoxide Hotels"

Diffractometers

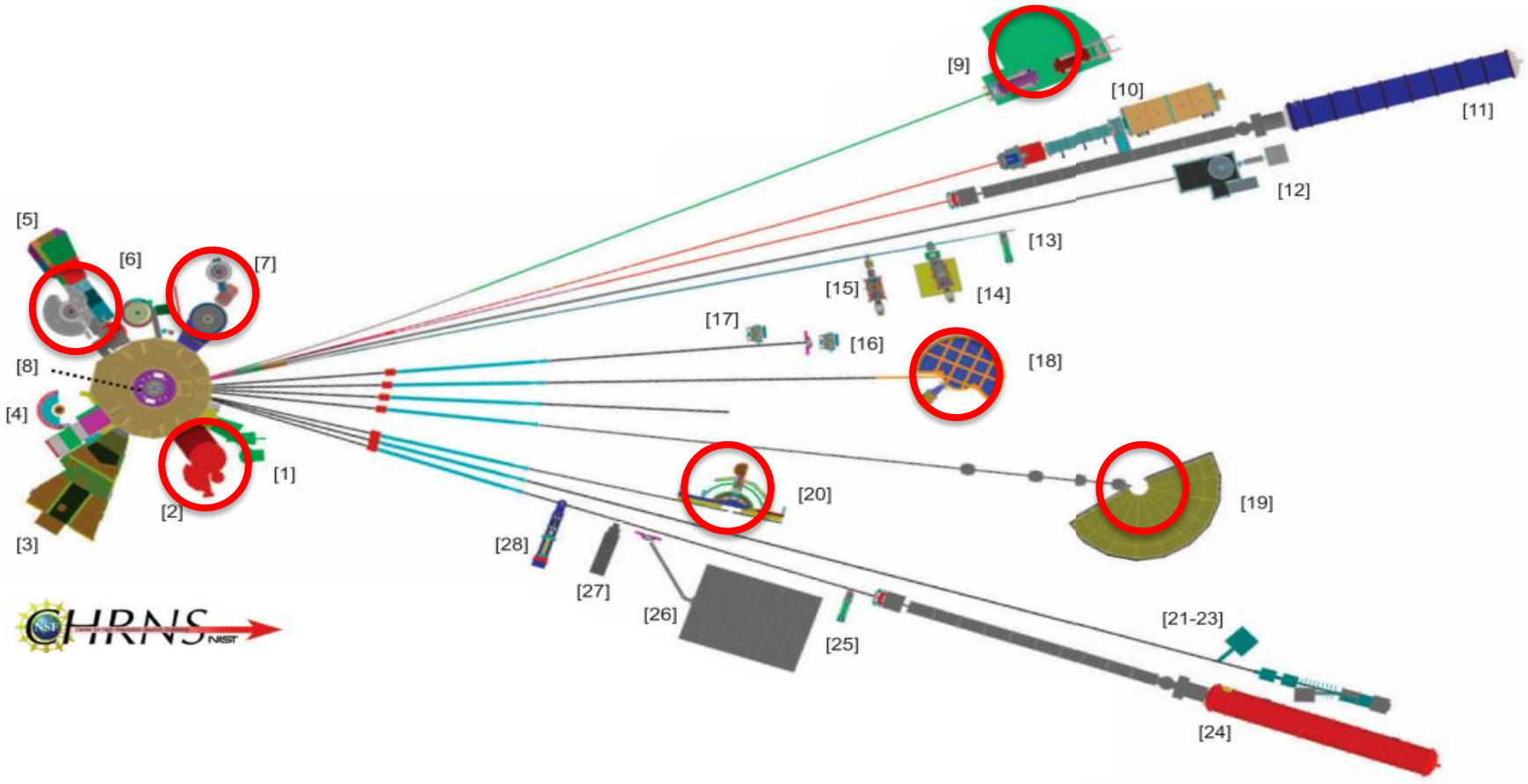


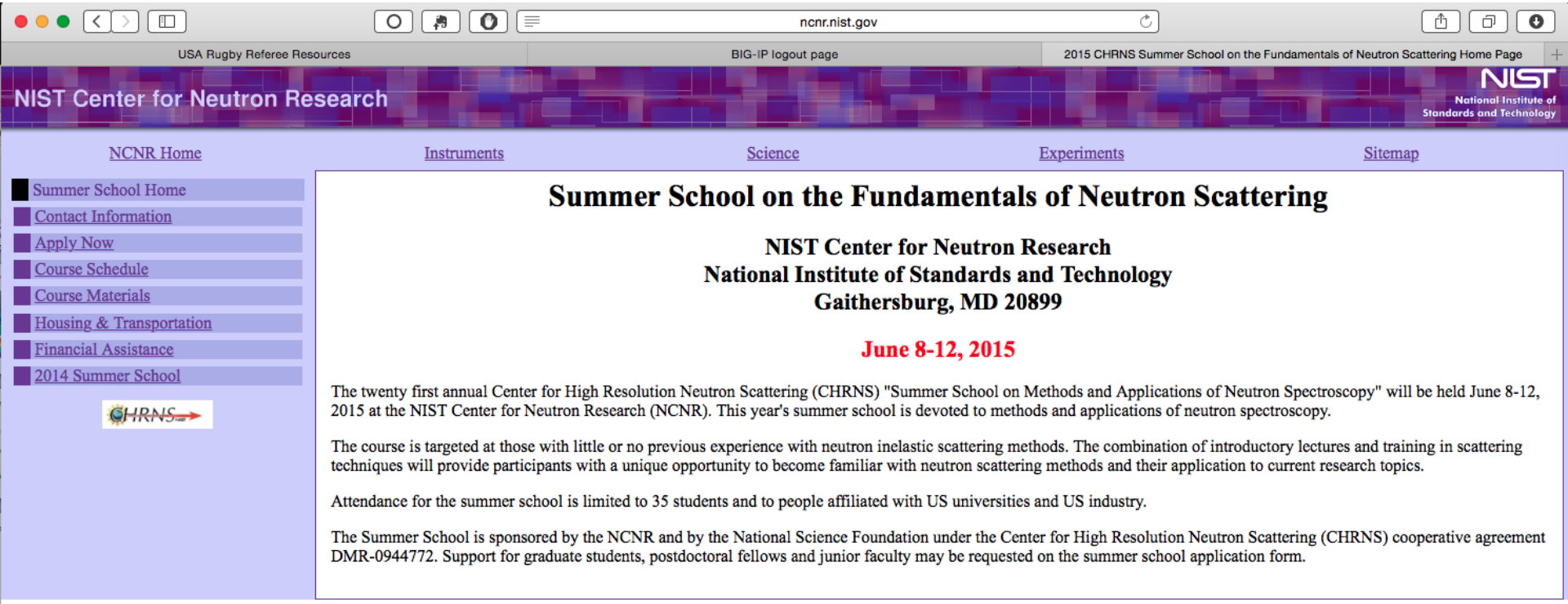


Bloch et al., J. Am. Chem. Soc. 2014

JACS Spotlight “Molecular Boxes Act like Little Carbon Monoxide Hotels"

Spectrometers





* Brought to you by NCNR and NSF