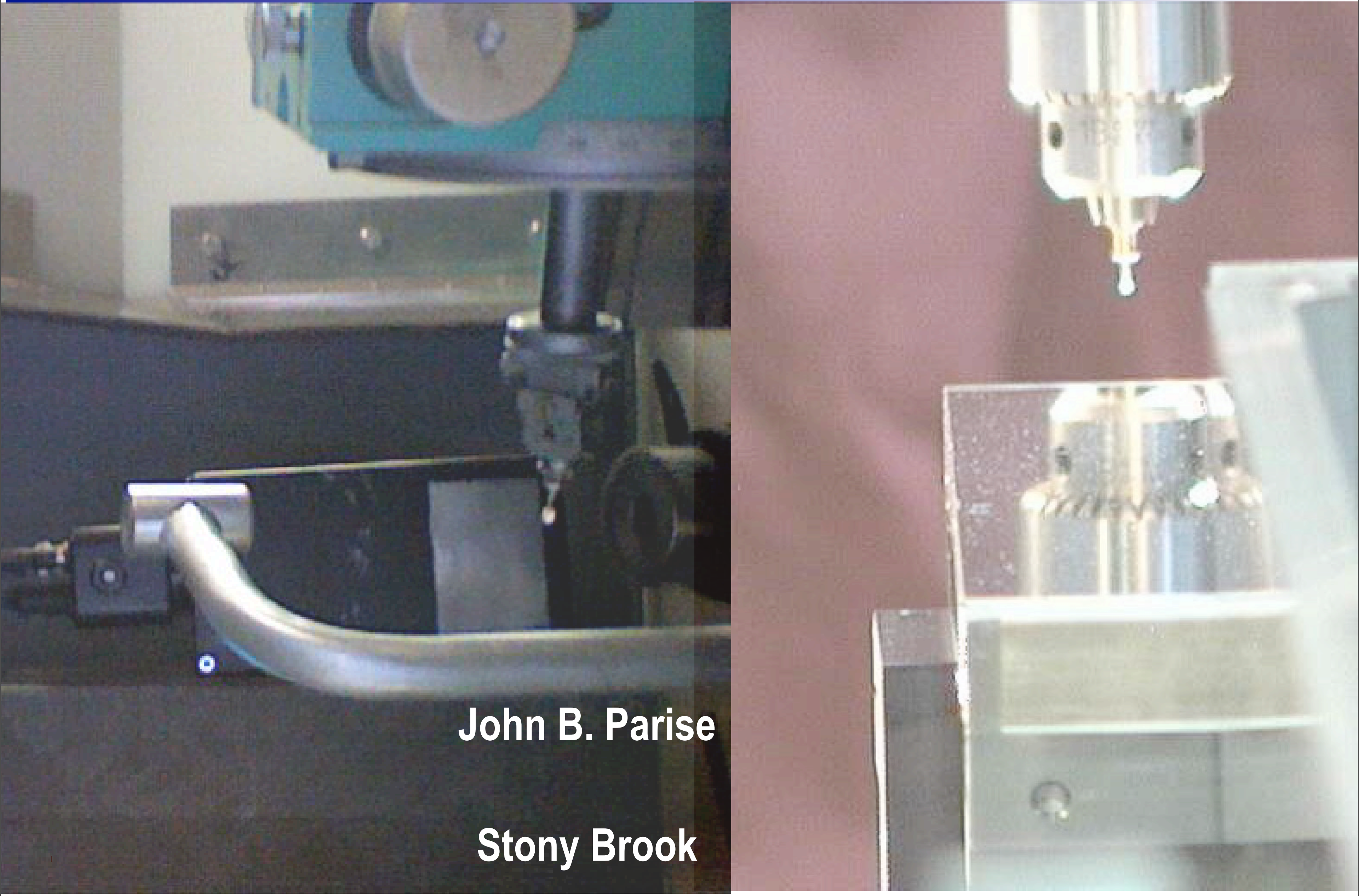
# Introduction to neutron science



**John B. Parise**

**Stony Brook**

# Outline

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- Why neutrons?
  - Properties of neutron (esp. compared to X-rays)
  - Consequences and applications
  - Scientific opportunities

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- Slow: $v \approx 4000$ m/s / ($\lambda$ / Å) and E distribution easily shifted
  - Same source - large E-range = many apps
  - Low energy, $E = mv2/2 \approx 82$ meV /($\lambda$2/Å2)
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- Neutrons have moments - interaction with unpaired electrons
    - Spin 1/2 -- same as unpaired electron - magnetism

# How do neutrons interact with atoms?

- *Neutron – nucleus interactions*
  - *Most probable interaction*
  - *Short range - essentially point scattering*
- *Neutron – electron interactions*
  - *Spin-spin interaction (requires unpaired electrons)*
  - **Magnetic scattering**

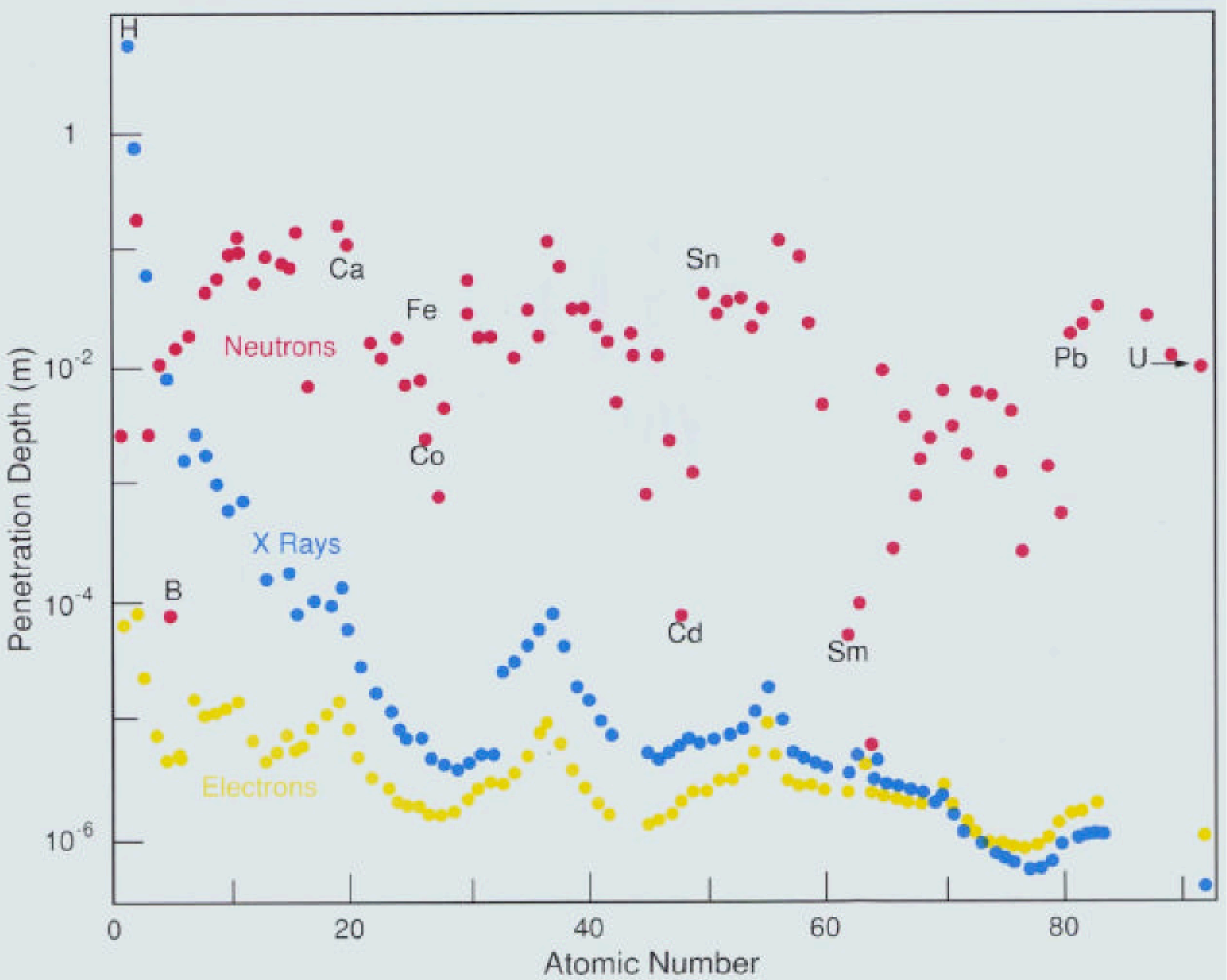
# When a Neutron Collides with an Atom Nucleus…

- **Neutron is absorbed - radiography**
  - yielding a new isotope (stable or radioactive)
  - to yield an excited nuclear state
- Neutron is scattered (momentum change)
  - Energy can be lost/gained (inelastic)
  - No energy transfer (elastic)

  *Also*
  - Phase can be lost (incoherent)
  - Phase can be retained (coherent)

# Properties - charge

- Neutral - no interaction with Coulomb charge
  - Highly penetrating



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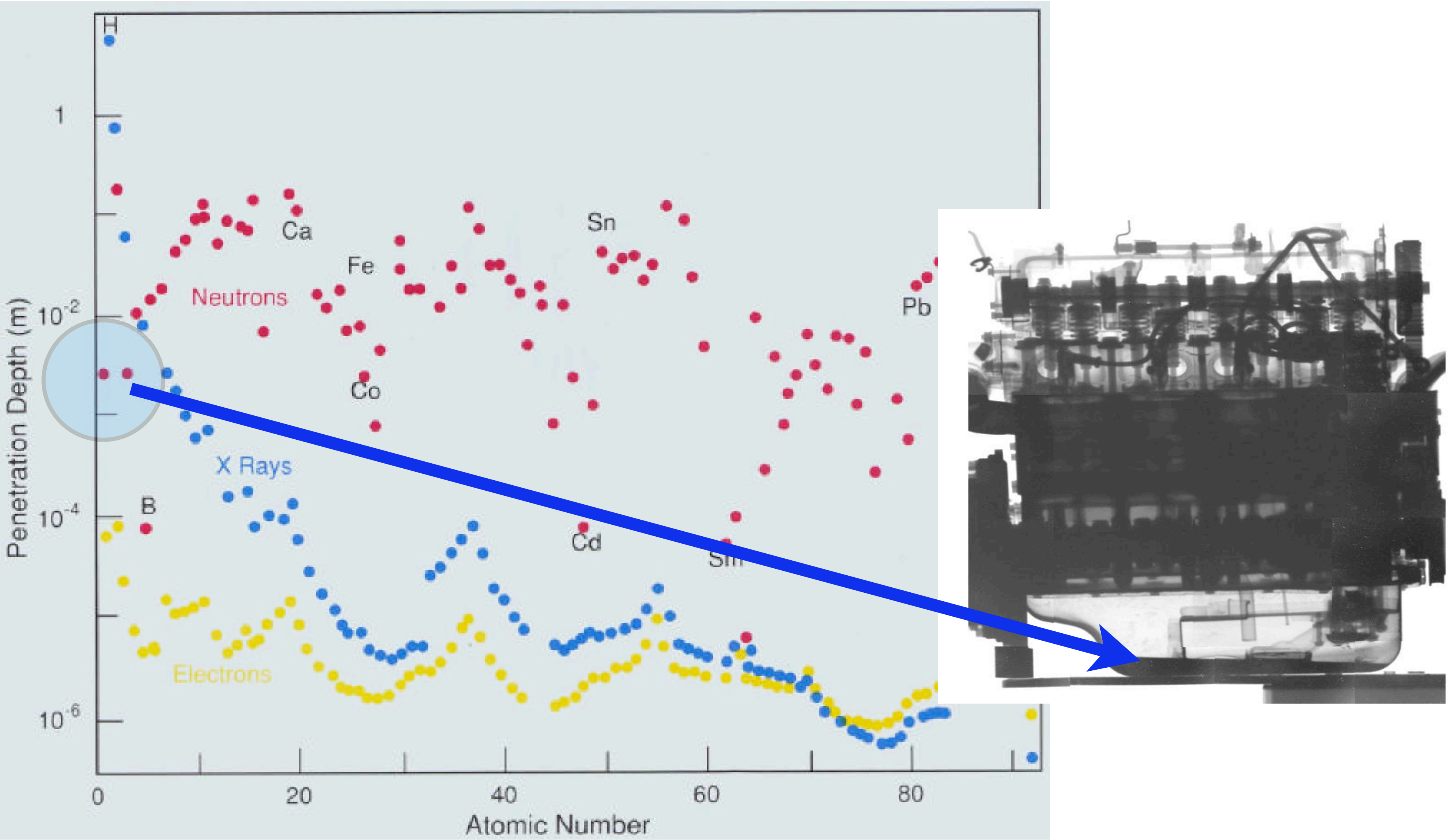

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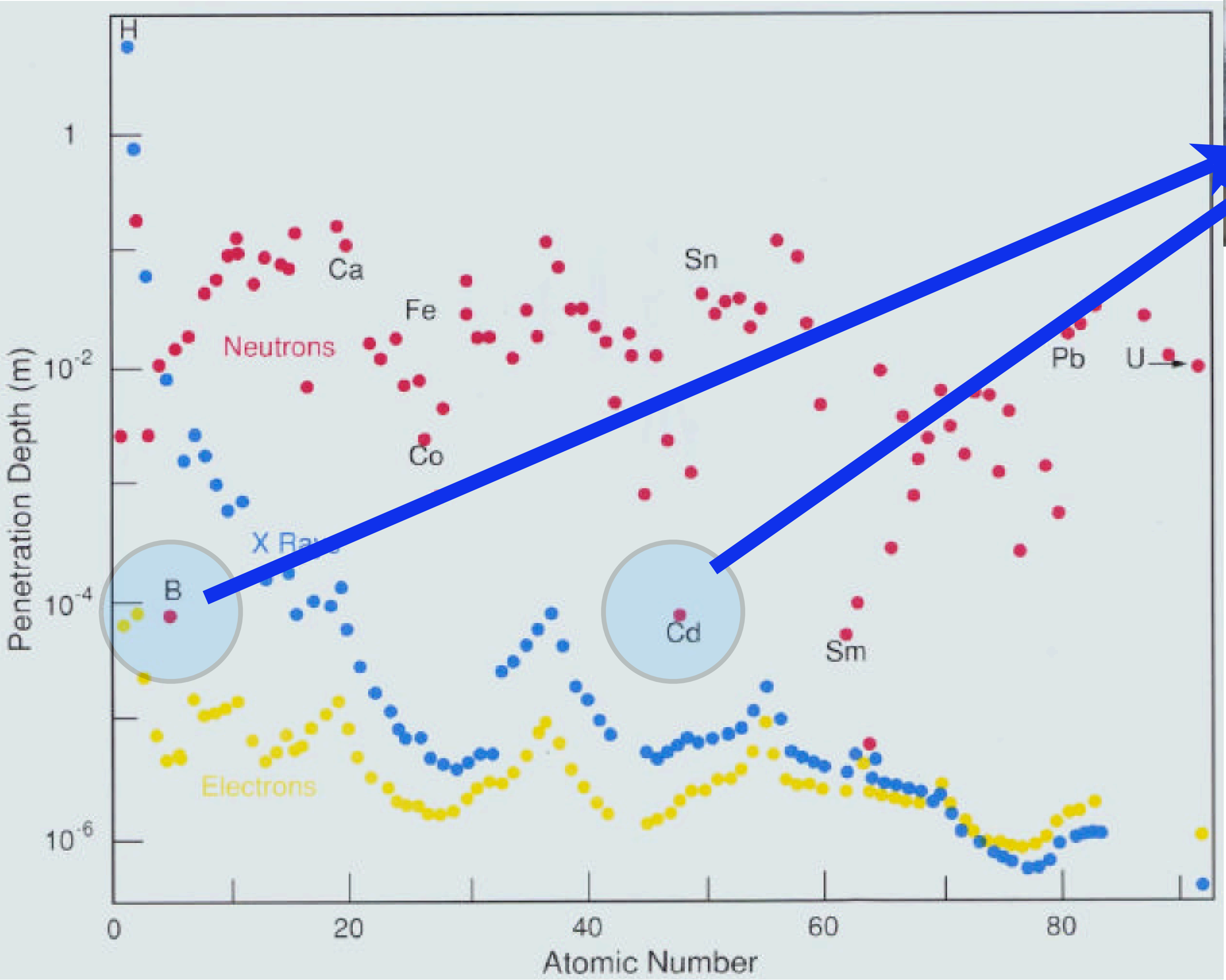

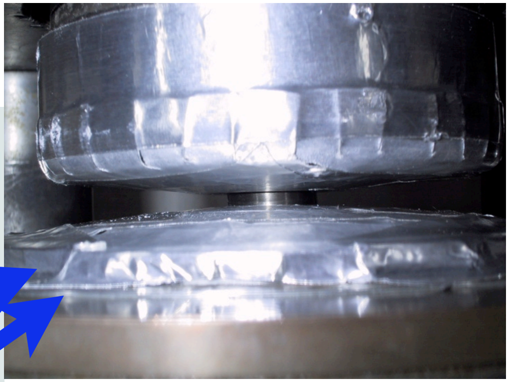

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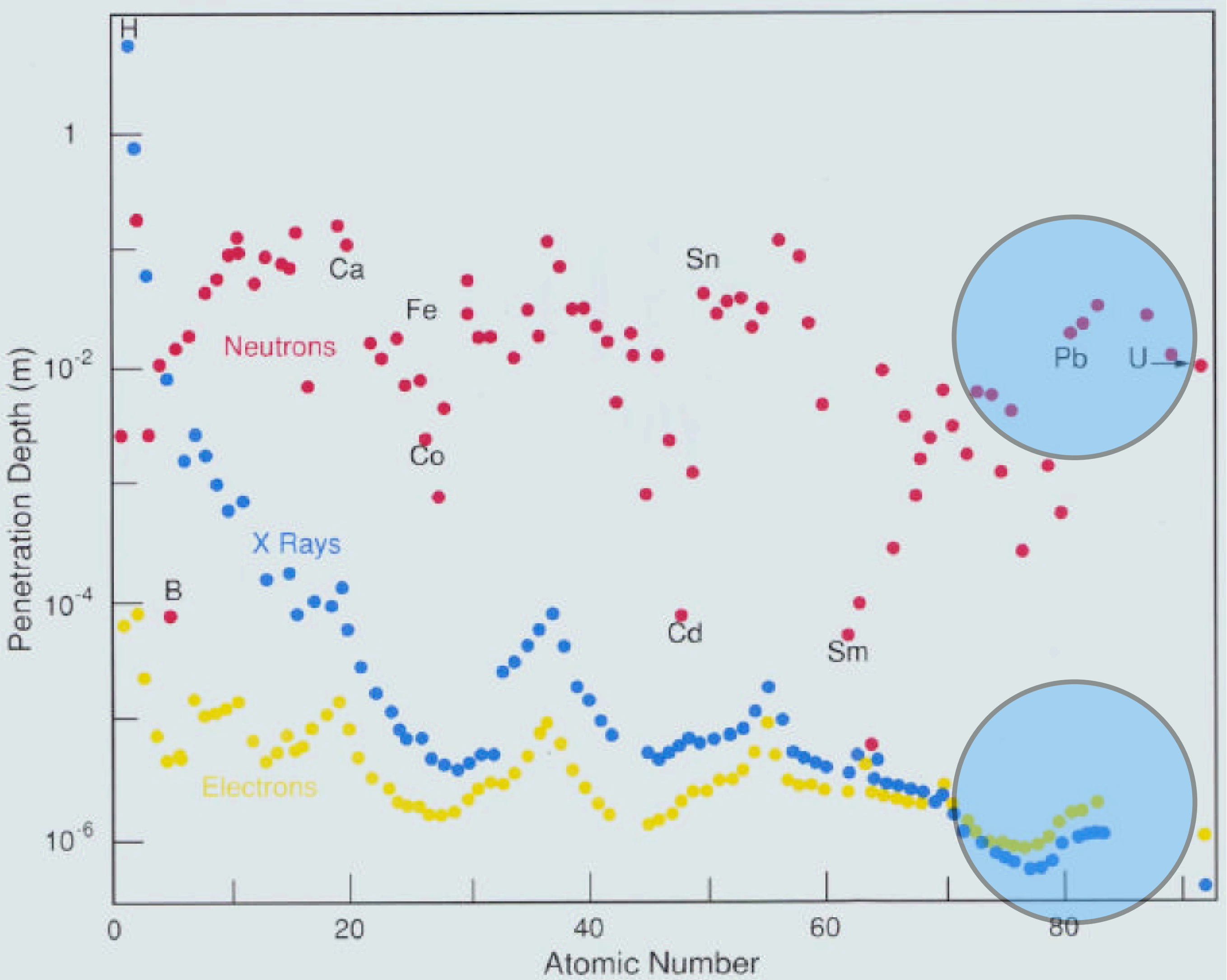
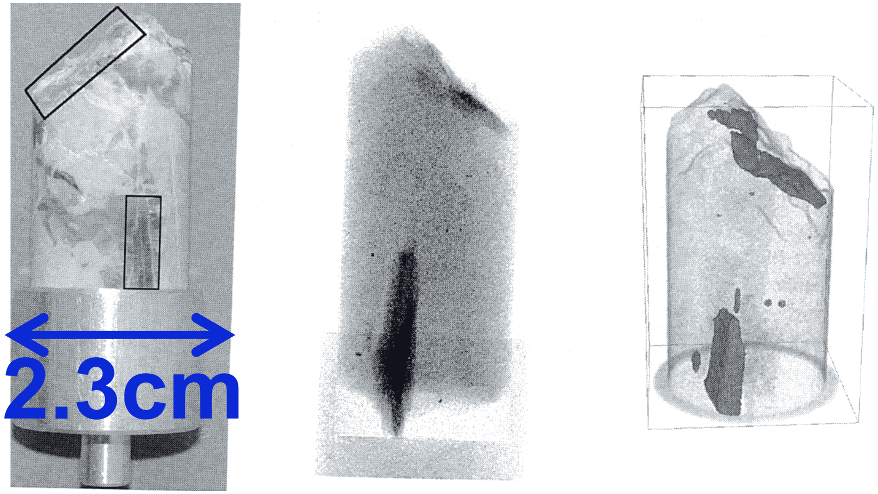
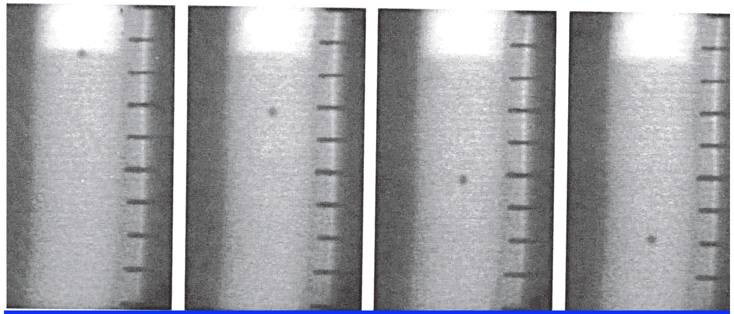


# Properties - charge

- Neutral - no interaction with Coulomb charge
  - Highly penetrating (except B, Cd, Gd, Hf ...)
- Applications
  - light-weight machinable shielding (BN); opaque self collimating anvils (c-BN); Imaging real rocks and parts



Neutrons penetrate deep into matter (Winkler et al, EJ Mineral., V14)



Radiographic images of highly Absorbing Hf sphere falling in silicate melt

# When a Neutron Collides with an Atom Nucleus…

- Neutron is absorbed
  - yielding a new isotope (stable or radioactive)
  - to yield an excited nuclear state - Neutron Activation Analysis
- Neutron is scattered (momentum change)
  - Energy can be lost/gained (inelastic)
  - No energy transfer (elastic)

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# Neutron activation analysis (NAA)

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- Expose sample + standards to neutrons.
  - most elements become radioactive.
  - Wait or measure while sample in beam (prompt γ - “neutron fluorescence”)
  - E of γ allows ID of element
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- Radiochemical NAA
  - Activation + separation of species of interest
  - low background, remove interference

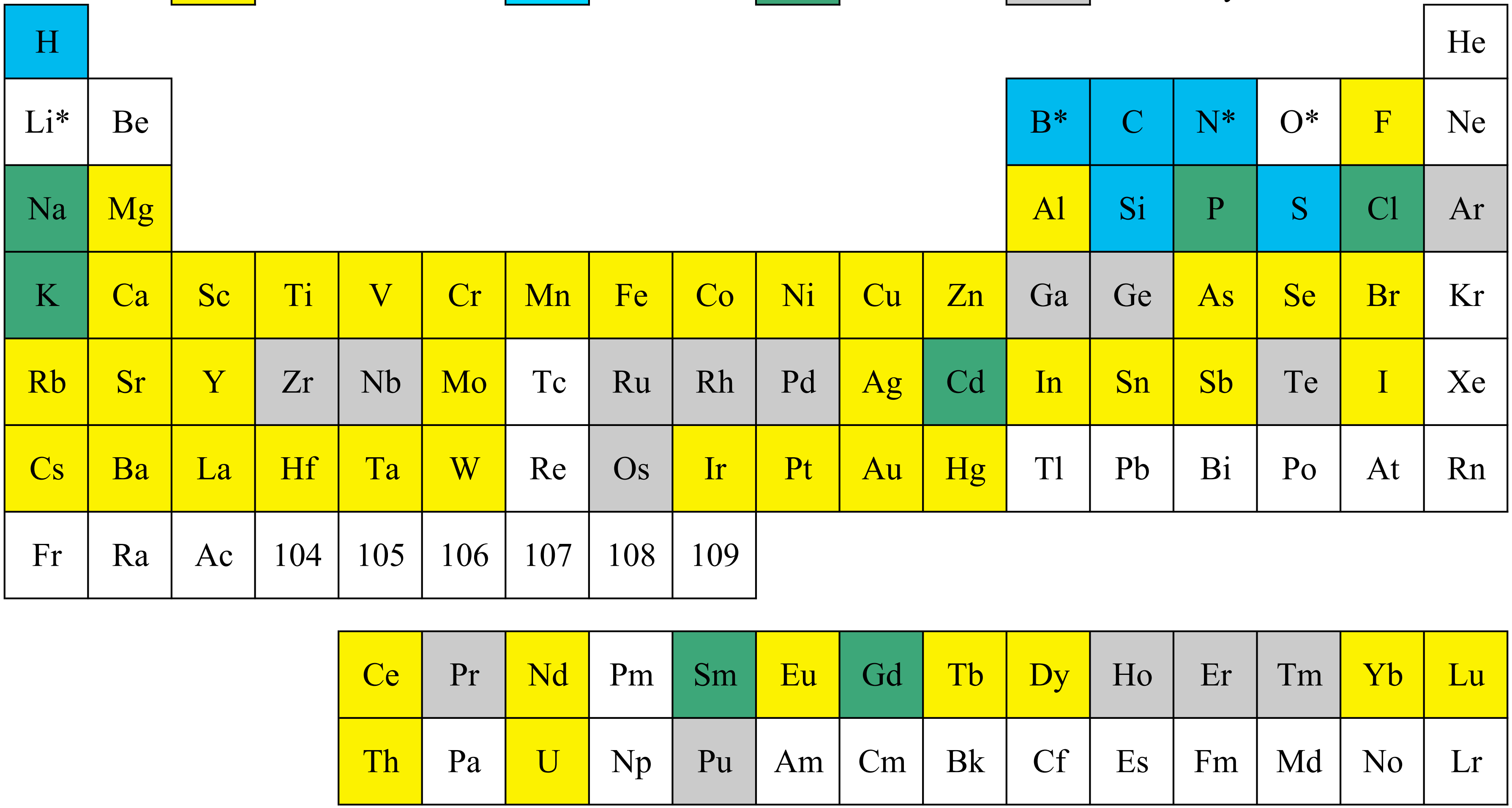
# Elements Determined Using Nuclear Analytical Methods

🟨 INAA / RNAA

🟦 PGAA

🟩 Both

▨ Potentially Measureable



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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 🟦 H | | | | | | | | | | | | | | | | | He |
| Li* | Be | | | | | | | | | | | 🟦 B* | 🟦 C | 🟦 N* | O* | 🟨 F | Ne |
| 🟩 Na | 🟨 Mg | | | | | | | | | | | 🟨 Al | 🟦 Si | 🟩 P | 🟦 S | 🟩 Cl | ▨ Ar |
| 🟩 K | 🟨 Ca | 🟨 Sc | 🟨 Ti | 🟨 V | 🟨 Cr | 🟨 Mn | 🟨 Fe | 🟨 Co | 🟨 Ni | 🟨 Cu | 🟨 Zn | ▨ Ga | ▨ Ge | 🟨 As | 🟨 Se | 🟨 Br | Kr |
| 🟨 Rb | 🟨 Sr | 🟨 Y | ▨ Zr | ▨ Nb | 🟨 Mo | Tc | ▨ Ru | ▨ Rh | ▨ Pd | 🟨 Ag | 🟩 Cd | 🟨 In | 🟨 Sn | 🟨 Sb | ▨ Te | 🟨 I | Xe |
| 🟨 Cs | 🟨 Ba | 🟨 La | 🟨 Hf | 🟨 Ta | 🟨 W | Re | ▨ Os | 🟨 Ir | 🟨 Pt | 🟨 Au | 🟨 Hg | Tl | Pb | Bi | Po | At | Rn |
| Fr | Ra | Ac | 104 | 105 | 106 | 107 | 108 | 109 | | | | | | | | | |
| | | | | | | | | | | | | | | | | | |
| | | | | 🟨 Ce | ▨ Pr | 🟨 Nd | Pm | 🟩 Sm | 🟨 Eu | 🟩 Gd | 🟨 Tb | 🟨 Dy | ▨ Ho | ▨ Er | ▨ Tm | 🟨 Yb | 🟨 Lu |
| | | | | 🟨 Th | Pa | 🟨 U | Np | ▨ Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No | Lr |

*NDP is used for surface analysis of B, Li, N, O.

Courtesy of Brian Toby, Argonne

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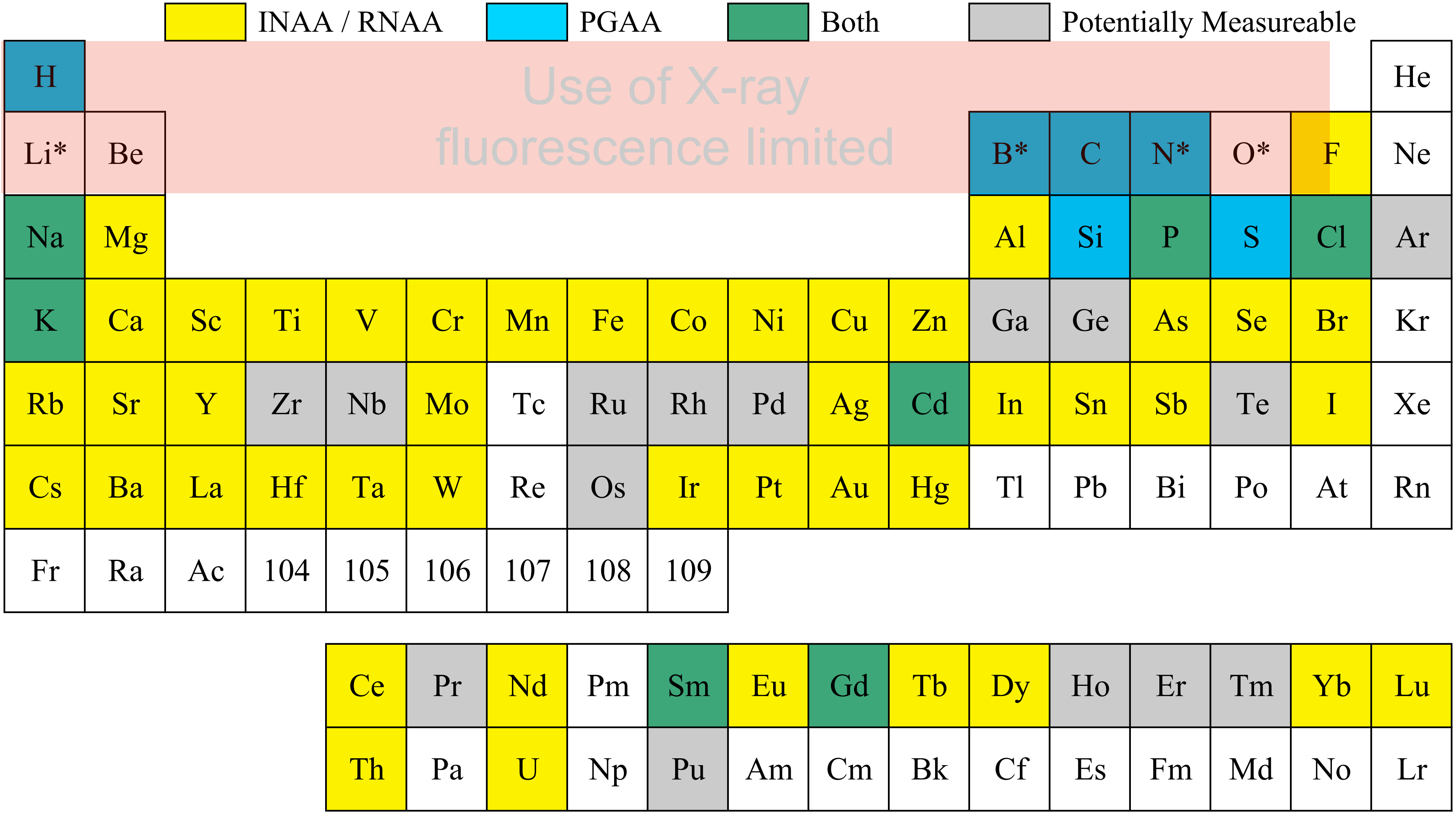

🟨 INAA / RNAA 🟦 PGAA 🟩 Both ▨ Potentially Measureable

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H 🟦 | | | | | | | | | | | | | | | | | He |
| Li* | Be | | | | | | | | | | | B* 🟦 | C 🟦 | N* 🟦 | O* | F 🟨 | Ne |
| Na 🟩 | Mg 🟨 | | | | | | | | | | | Al 🟨 | Si 🟦 | P 🟩 | S 🟦 | Cl 🟩 | Ar ▨ |
| K 🟩 | Ca 🟨 | Sc 🟨 | Ti 🟨 | V 🟨 | Cr 🟨 | Mn 🟨 | Fe 🟨 | Co 🟨 | Ni 🟨 | Cu 🟨 | Zn 🟨 | Ga ▨ | Ge ▨ | As 🟨 | Se 🟨 | Br 🟨 | Kr |
| Rb 🟨 | Sr 🟨 | Y 🟨 | Zr ▨ | Nb ▨ | Mo 🟨 | Tc | Ru ▨ | Rh ▨ | Pd ▨ | Ag 🟨 | Cd 🟩 | In 🟨 | Sn 🟨 | Sb 🟨 | Te ▨ | I 🟨 | Xe |
| Cs 🟨 | Ba 🟨 | La 🟨 | Hf 🟨 | Ta 🟨 | W 🟨 | Re | Os ▨ | Ir 🟨 | Pt 🟨 | Au 🟨 | Hg 🟨 | Tl | Pb | Bi | Po | At | Rn |
| Fr | Ra | Ac | 104 | 105 | 106 | 107 | 108 | 109 | | | | | | | | | |
| | | | | | | | | | | | | | | | | | |
| | | | | Ce 🟨 | Pr ▨ | Nd 🟨 | Pm | Sm 🟩 | Eu 🟨 | Gd 🟩 | Tb 🟨 | Dy 🟨 | Ho ▨ | Er ▨ | Tm ▨ | Yb 🟨 | Lu 🟨 |
| | | | | Th 🟨 | Pa | U 🟨 | Np | Pu ▨ | Am | Cm | Bk | Cf | Es | Fm | Md | No | Lr |

Use of X-ray fluorescence limited

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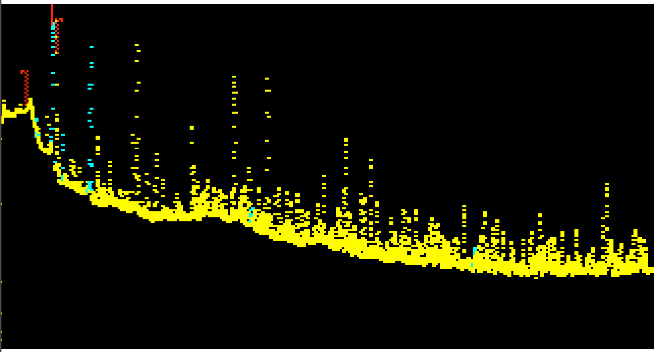
# NIST: SRM 695 Trace Elements in Multi-Nutrient Fertilizer



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**Cd Hg As Se Zn**

**Ni Pb Cu Mo Co**

Background: In 1998, percent levels of Cd were found in a chemical fertilizer that was applied to farmland in California. Many states proposed regulations limiting levels of 10 elements shown above. Fertilizer manufacturers and state regulators needed standards to develop methods and validate analytical results.

Project: Material was donated by the industry. Sieved fractions were analyzed by INAA and the decision was made to jet mill the material. XRF and PGAA were used to assess homogeneity of the final material.

Certification analyses underway in FY05. **Certified or reference values planned for 23 elements, 19 to be determined by nuclear methods**

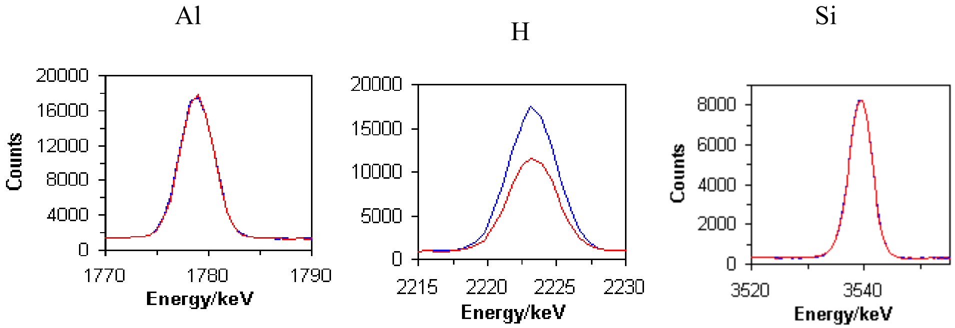
# Prompt-$\gamma$ Activation Analysis

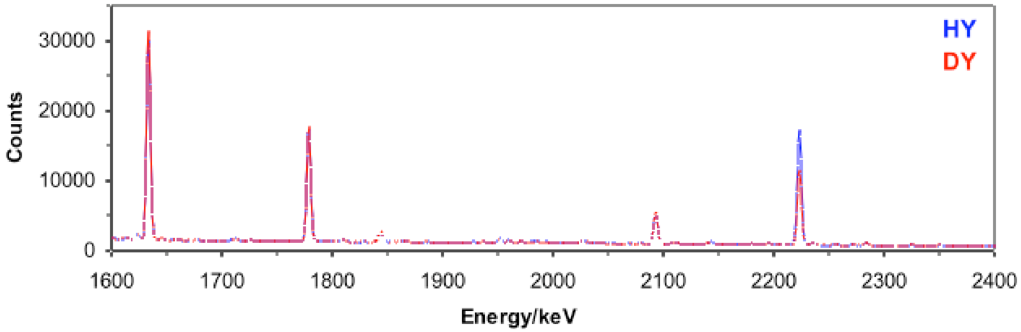
- **non-destructive analytical chemistry Detects ~1/3 of periodic table**
  - **ppm sensitivity for hydrogen**

*Example:* Attempted deuteration of HY (Fajasite)

$H_{0.28}Al_{0.28}Si_{0.72}O_2$ vs

“$D_{0.28}Al_{0.28}Si_{0.72}O_2$”





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  *Also*

  - Phase can be lost (incoherent) - no interference (diffraction) effects
  - Phase can be retained (coherent) - interference between scattering centers - diffraction effects

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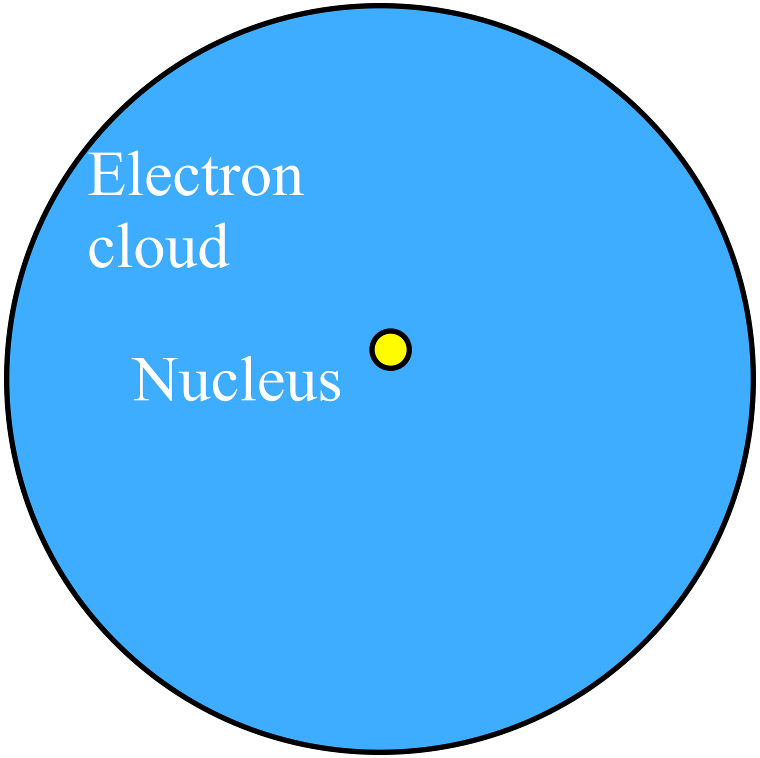
- Difference between X-ray and neutron cross-sections ($\sigma_{total}$)
  - While the cross-section (probability of scattering) is positive the atomic scattering length, b ($\sigma = 4\pi b^2$) can be negative
    - +ve b, scattered neutron $\pi/2$ phase shifted (like X-rays)
  - b is different for different isotopes, different nuclear spin states

# The Scattering (or X-ray or neutron) cross-section

- Other differences
  - The nucleus is a point compared to electron cloud
    - No dependence on scattering angle
    - the neutron interaction stay the same - and weak!



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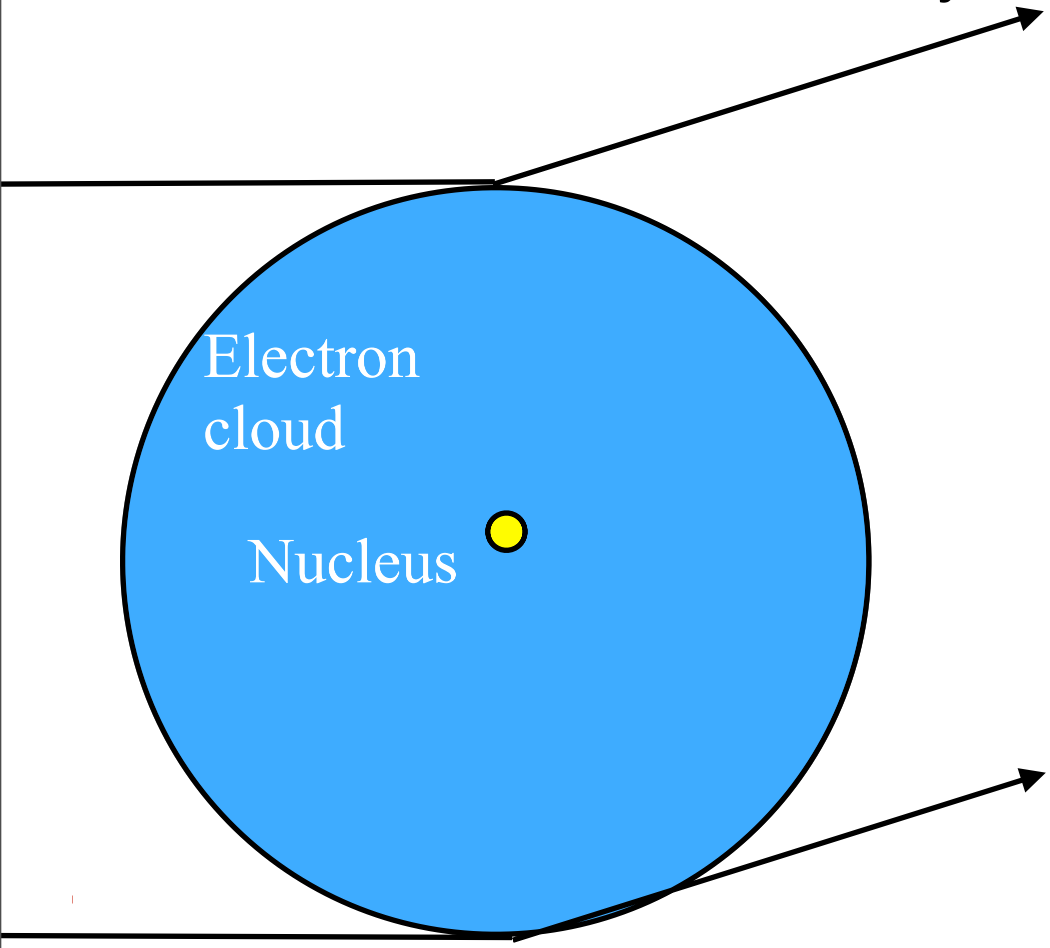

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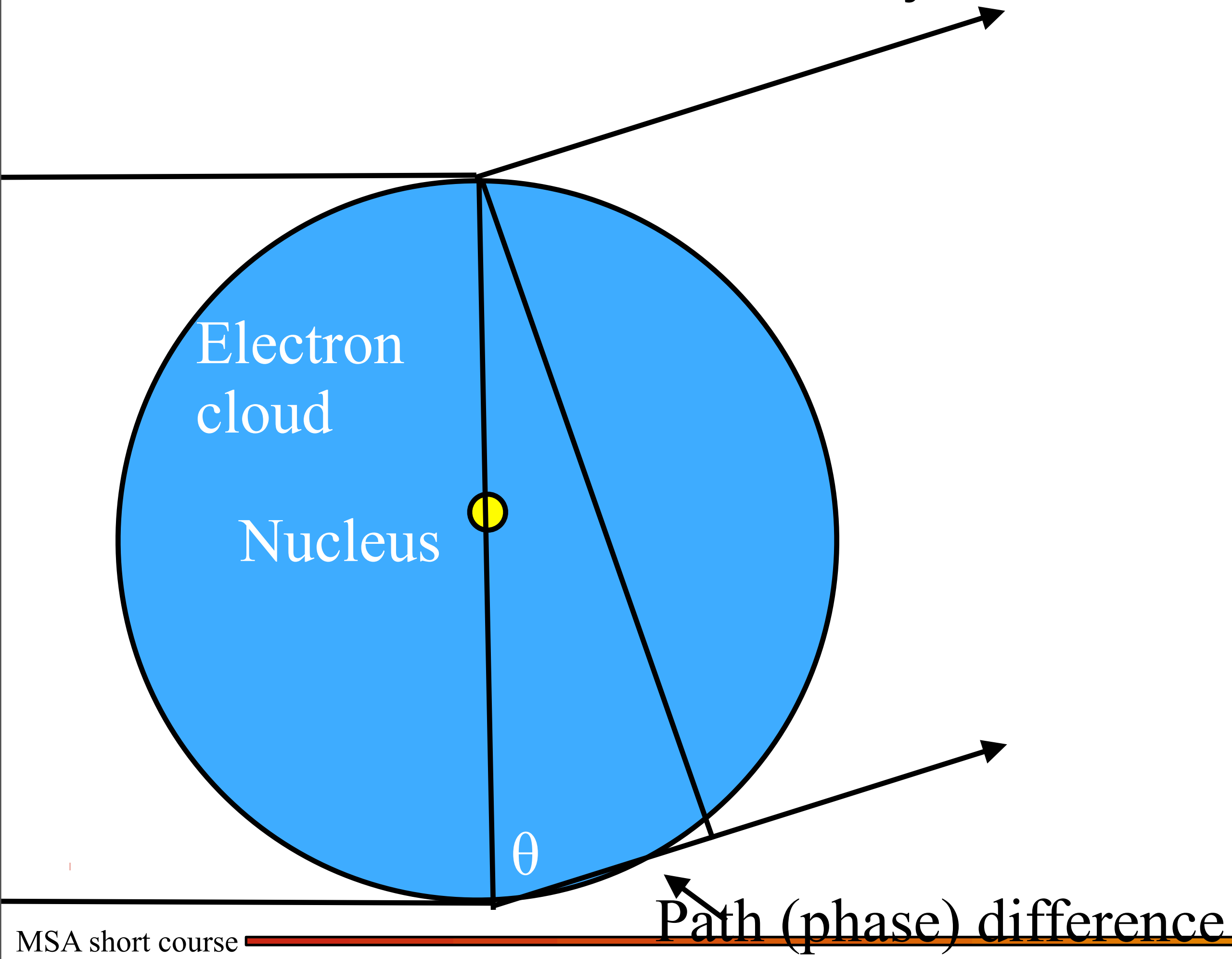

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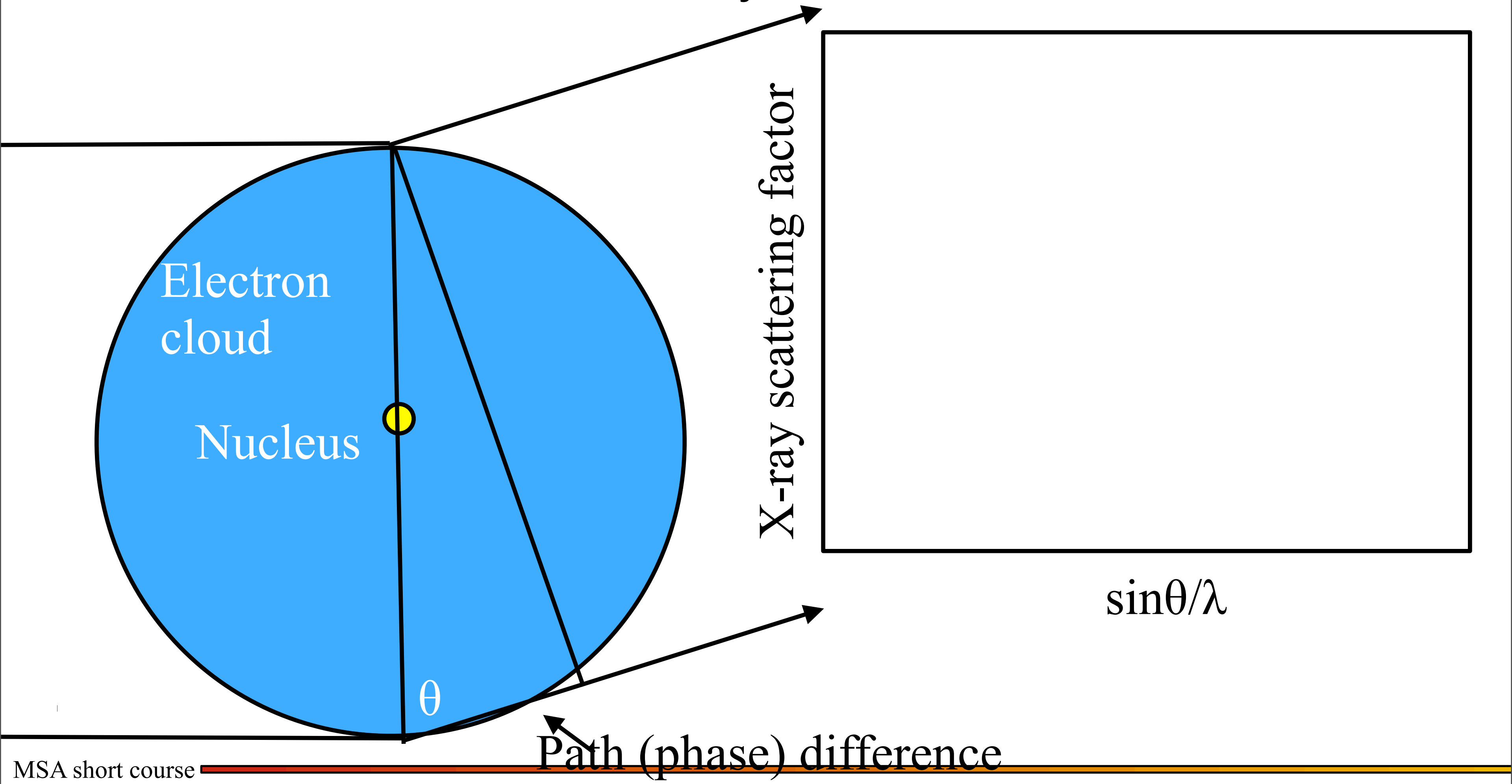

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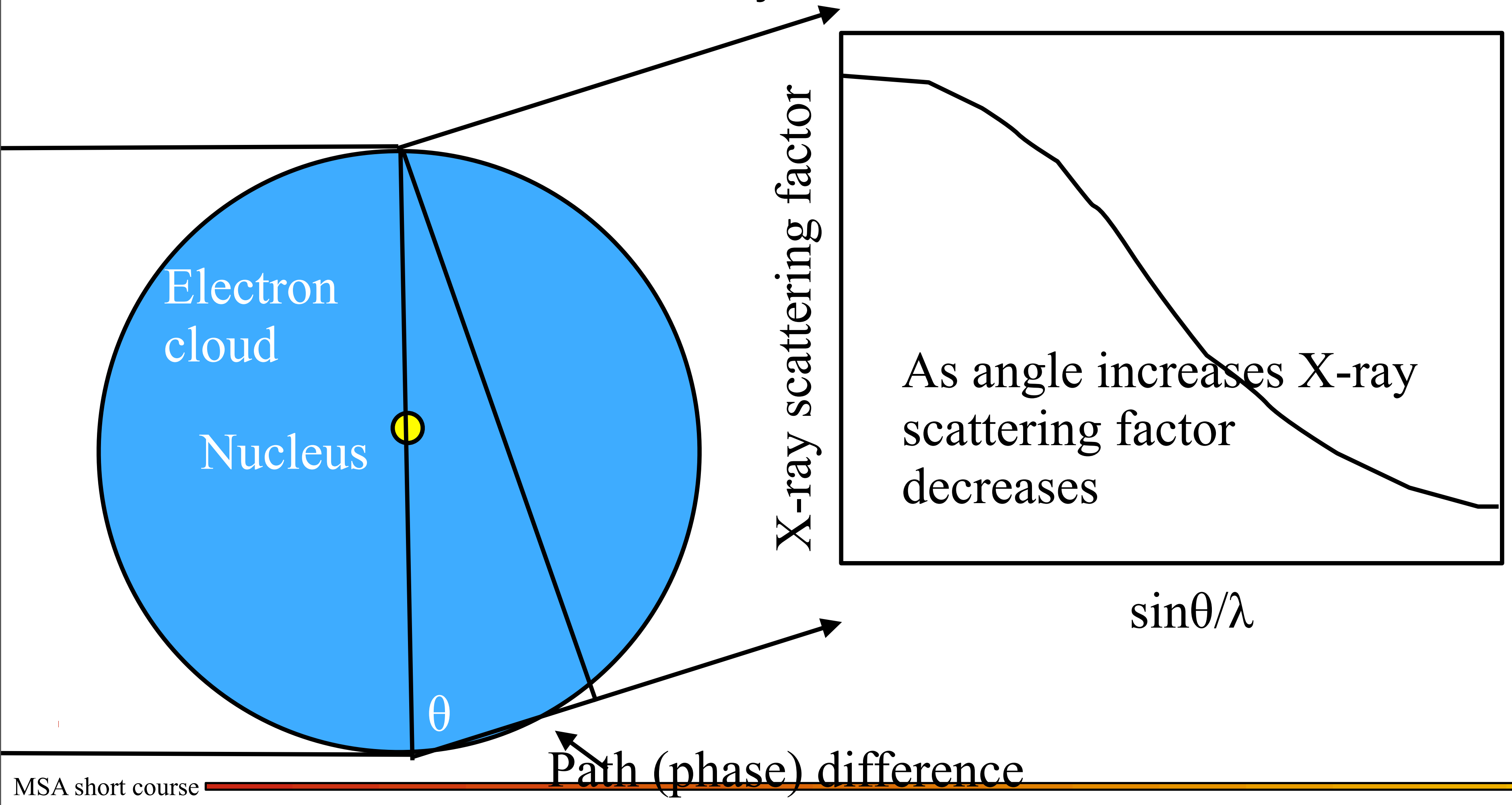


As angle increases X-ray scattering factor decreases

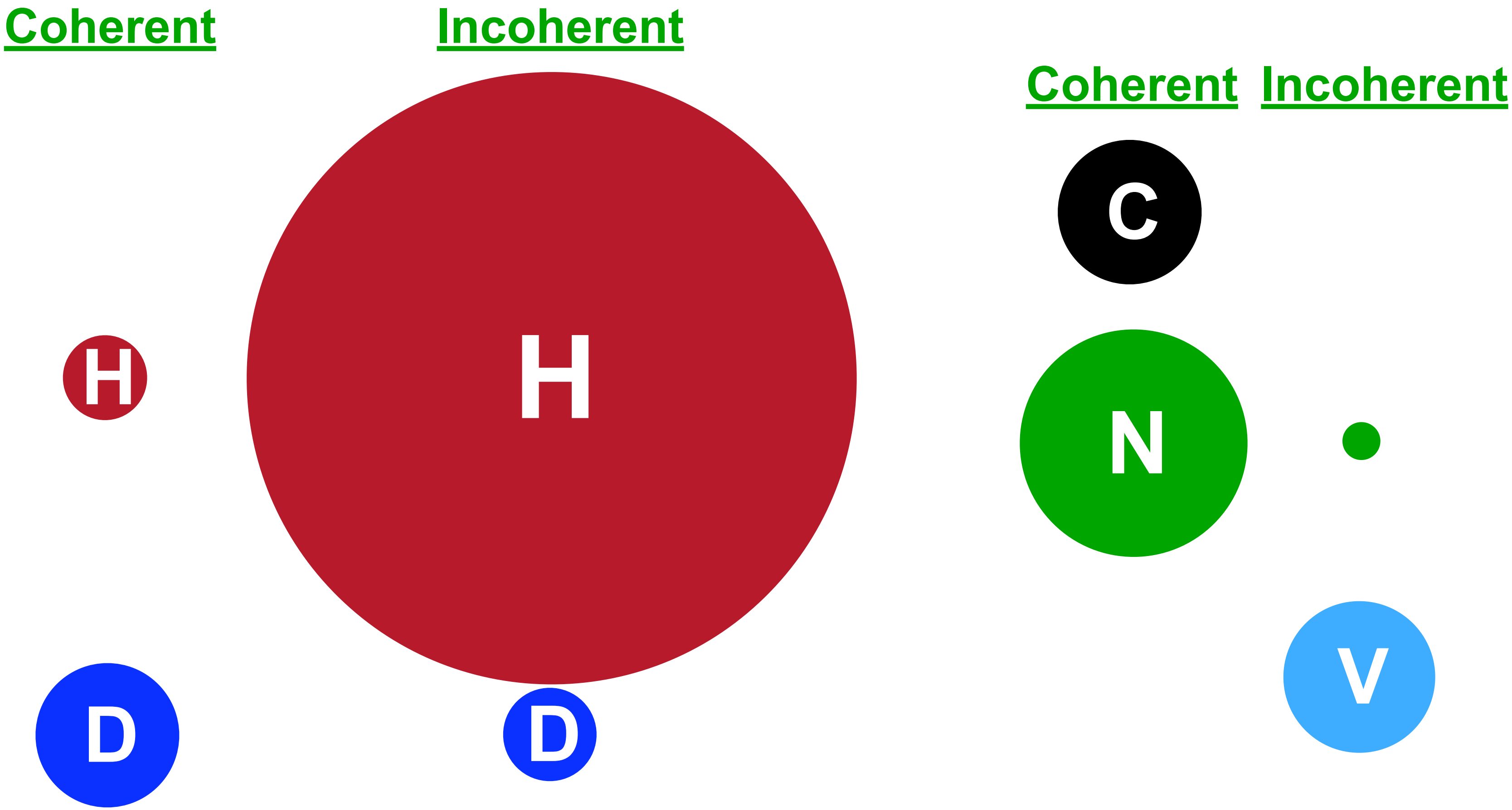
# The Scattering (or X-ray or neutron) cross-section

- Other differences
  - The nucleus is a point compared to electron cloud
    - No dependence on scattering angle
  - Can't be calculated; must be measured
  - Probability of coherent (phase retained, interference effects) and incoherent (phase lost) varies with isotope (not just atom)

$$\sigma_{coh} = 4\pi\left(\bar{b}\right)^2, \qquad \sigma_{inc} = 4\pi\left\{\overline{b^2} - \left(\bar{b}\right)^2\right\}$$

  - Coherent scattering depends on correlation between positions of nuclei, interference effects, Bragg, phonon scattering (correlated motion)
  - Incoherent scattering does not give rise to interference effects
    - Useful in studies of diffusion (uncorrelated motion), since it arises from correlations of the same nucleus at different times.

# Probability for coherent vs. incoherent scattering changes with isotope



Coherent Incoherent

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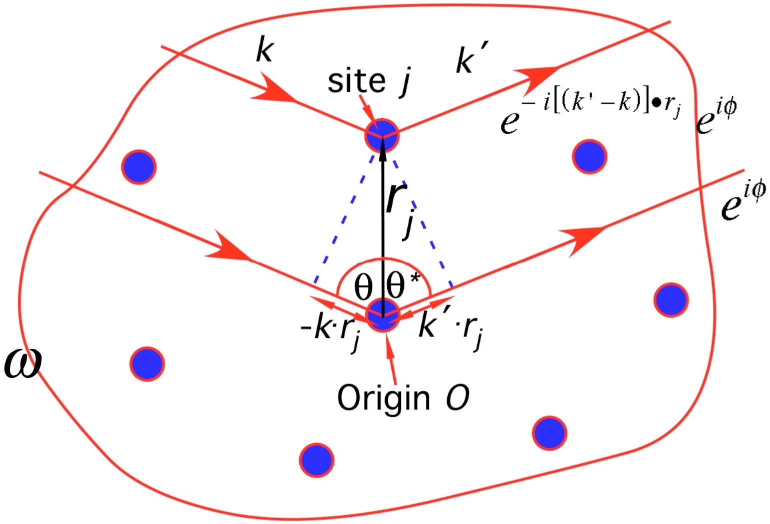
# Van Hove's scattering "law": periodic structure or not

## calculate this, exactly

$$\left(\frac{d^2\sigma}{d\omega dE'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}NS(Q,\omega)$$

$$S(Q,\omega) = \frac{1}{2\pi\hbar}\int G(r,t)\exp\{(i(Q\cdot r-\omega t)\}\ \mathrm{d}r\ \mathrm{d}t$$

$$G(r,t) = \frac{\hbar}{(2\pi)^3}\int S(Q,\omega)\exp\{(-i(Q\cdot r-\omega t)\}\ \mathrm{d}Q\ \mathrm{d}\omega$$



***G*(*r*, *t*) is the *time-dependent pair-correlation function* (*where the atoms are*)**

***S*(*Q*, ω) is the *structure* function, *dynamical structure function*, *coherent scattering function*, also referred to as the *scattering function* or scattering law. By inspection *S*(*Q*, ω) is the Fourier transform of *G*(*r*, *t*) in space and time (d*r* d*t*).**

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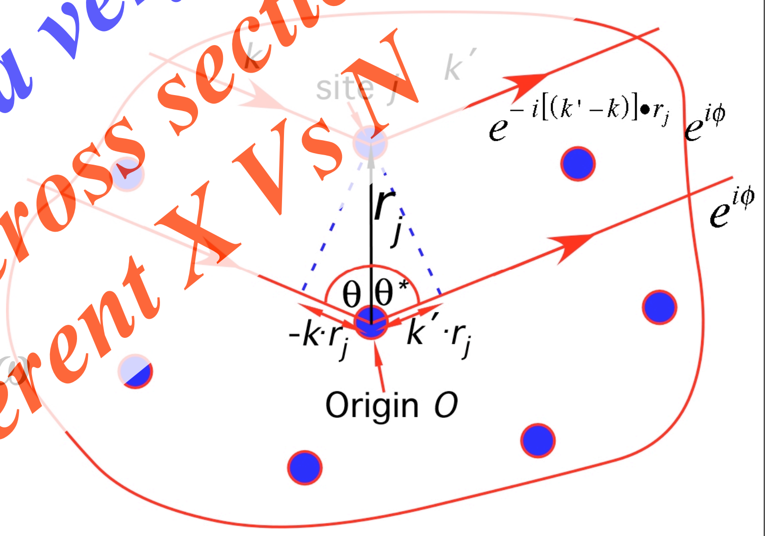
$$G(r,t) = \frac{\hbar}{(2\pi)^3}\int S(Q,\omega)\exp\{(-i(Q\cdot r-\omega t)\}\,dQ\,d\omega$$

**neutron’s (unlike X-rays) “sensitivity” almost equal at all Q and a very wide range of ω; coherent cross section, σ<sub></sub>**



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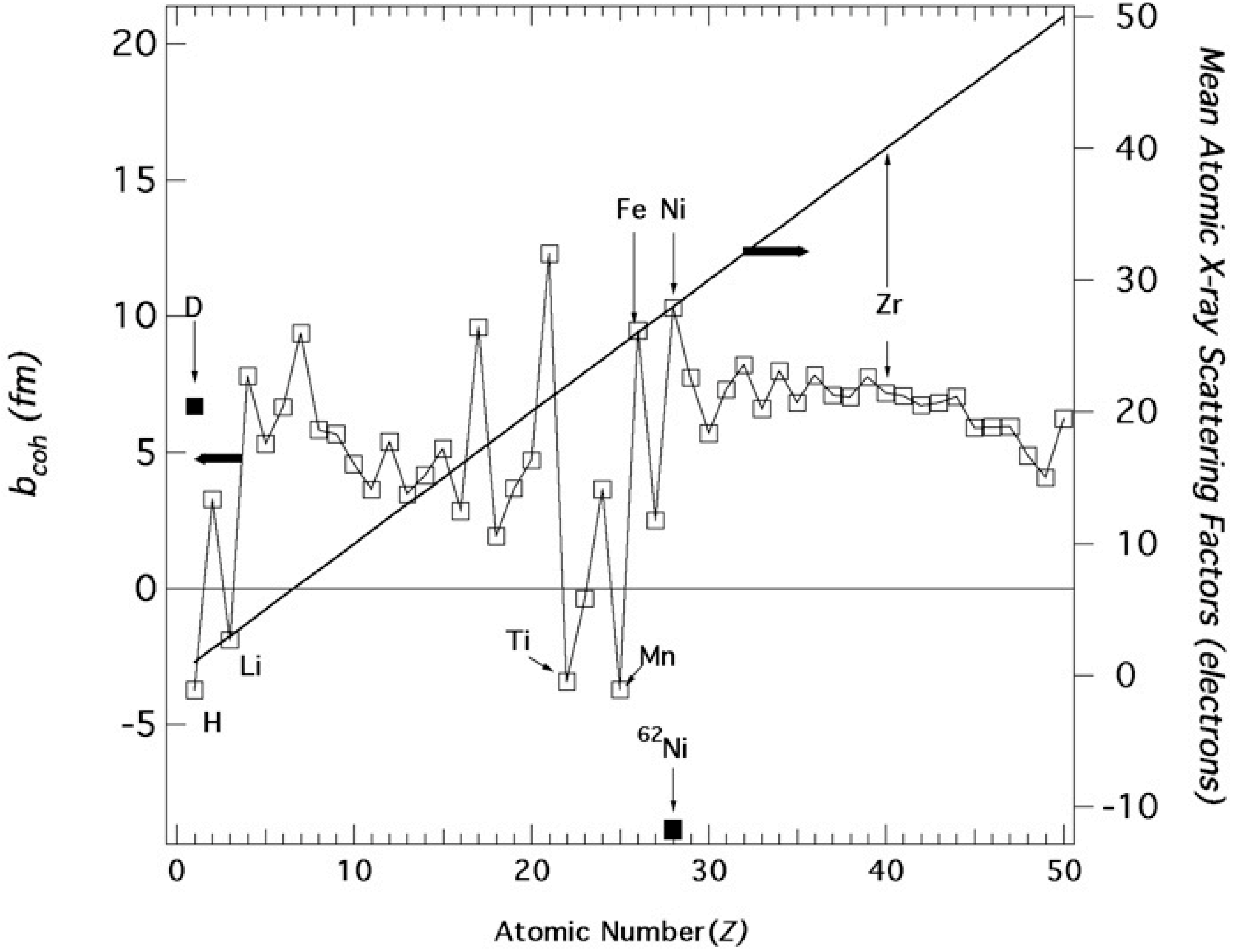
# Differences between X-ray and neutron cross-sections.
## (1) Z-dependence - Application: finding light elements



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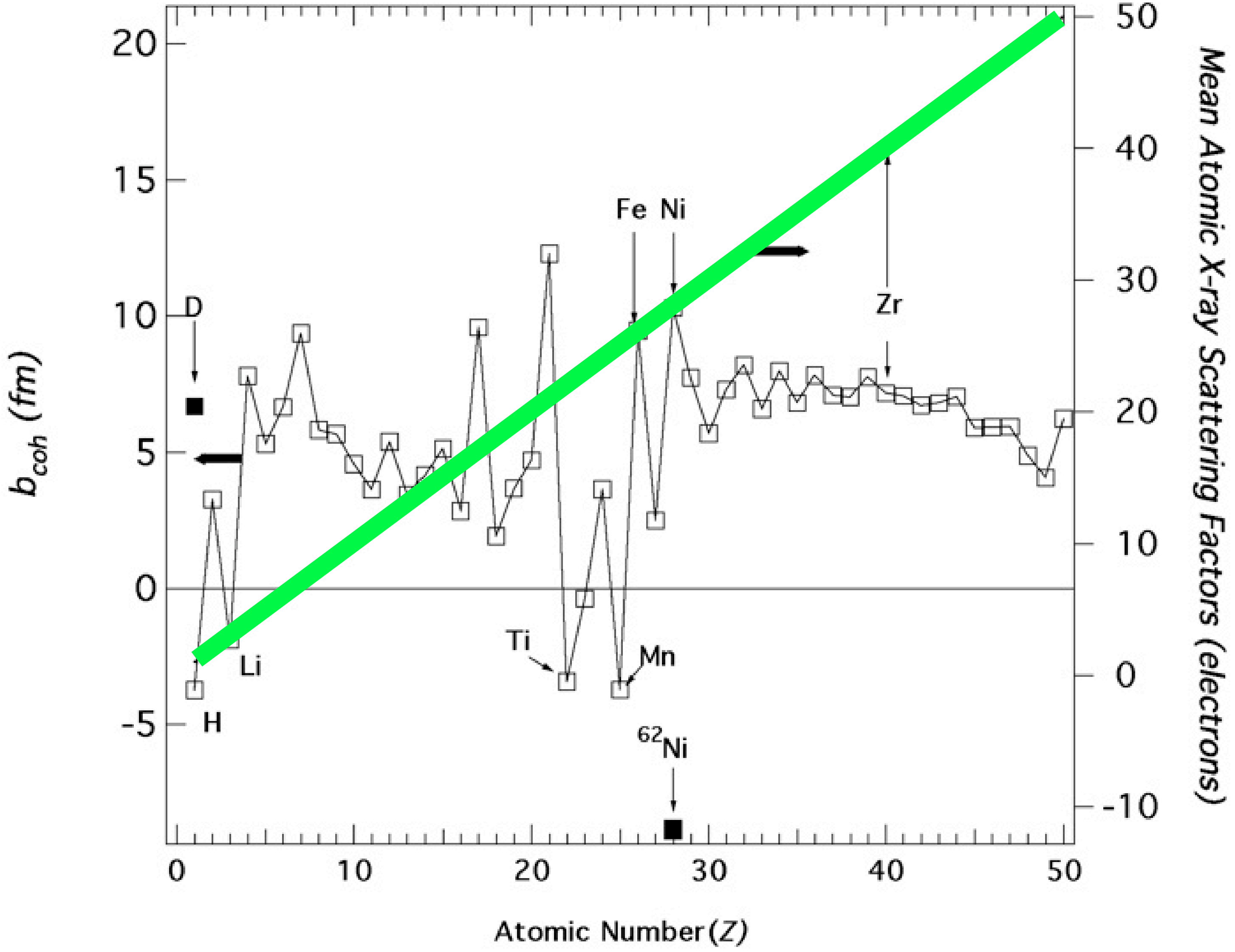

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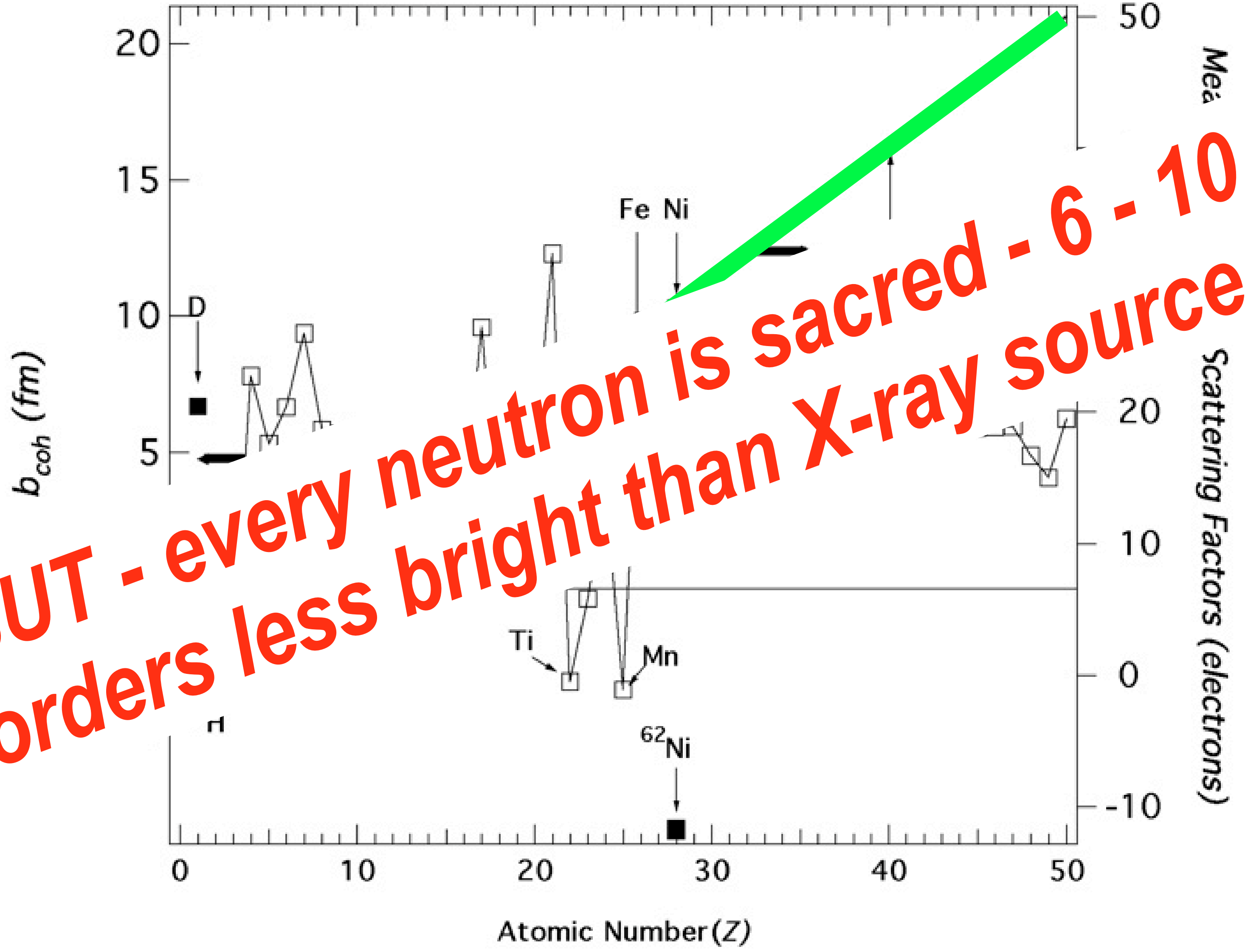

**BUT - every neutron is sacred - 6 - 10 orders less bright than X-ray sources.**

# Why Neutrons ?

- Neutrons are electrically neutral & more penetrating than X-rays.
  - tomography, radiography of real rocks and parts
- Neutrons act like particles
  - waveguides, gavitational effects
- Neutrons act like waves
  - Neutrons interact with nuclei & locate atoms more precisely.
    - Light atoms scatter neutrons as strongly as heavy atoms.
    - $b_{coh}$ independent of Z, $\sin\theta/\lambda$, can be -ve
    - Diffraction, D/H contrast, precise positions, PDF
- Neutrons have a moment, & can determine magnetic structures.

- Neutrons can study atom dynamics & the forces between atoms.

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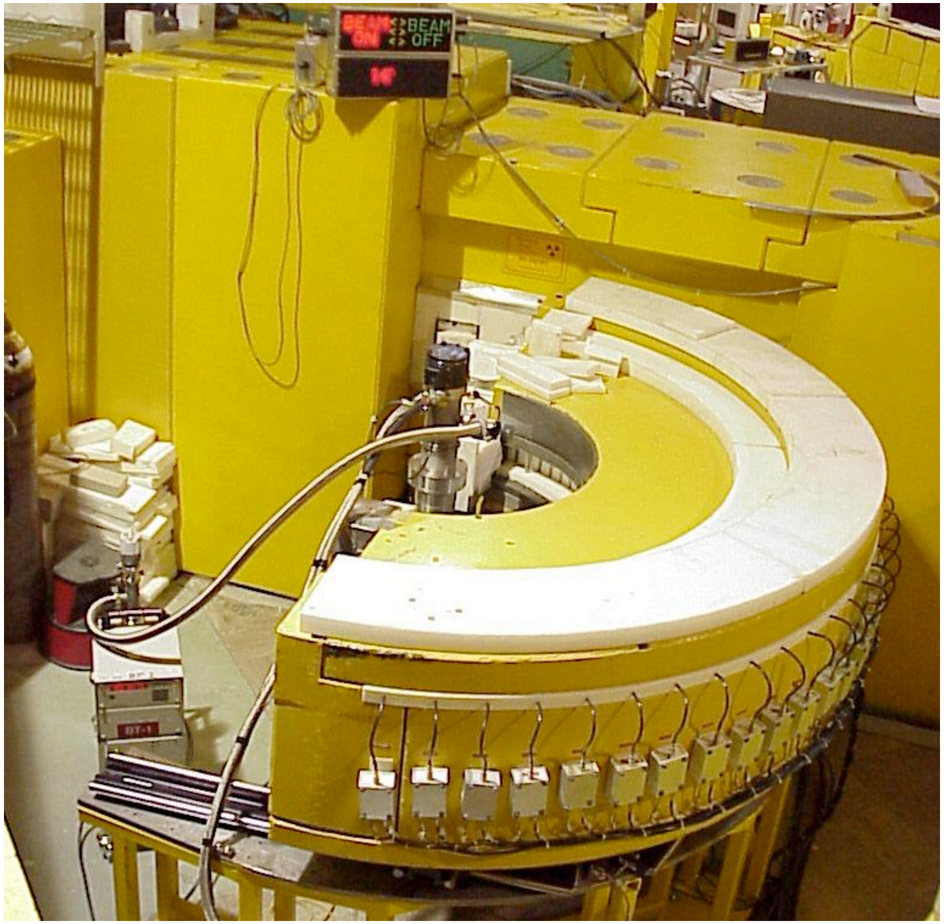
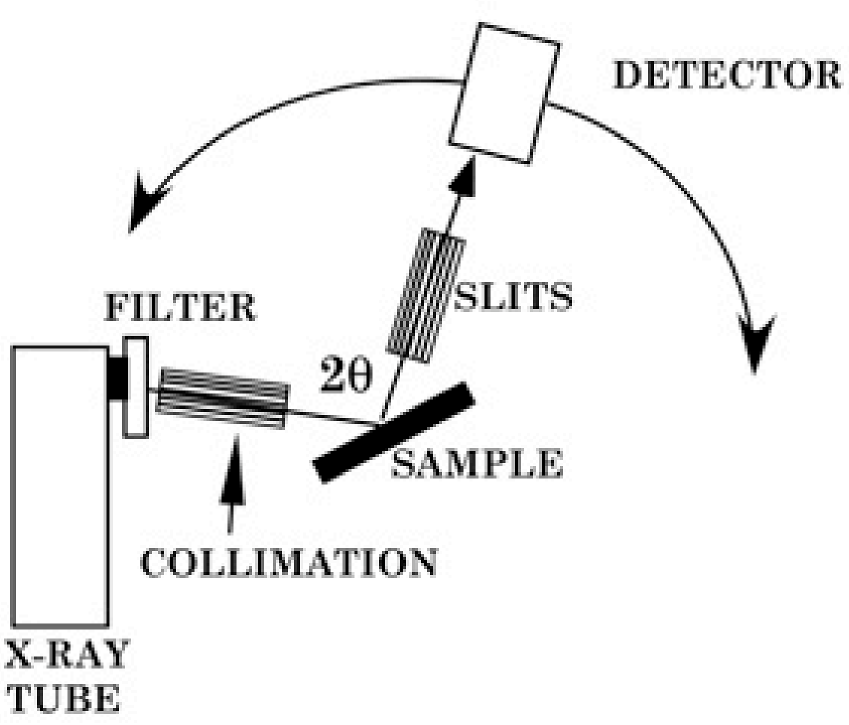
Application 1
- Bragg powder scattering - the experimental set-up looks familiar
- Data interpretation (peak position, unit cell, strain broadening, particle size effects, calculation of scattering factor) similar

# Properties of thermal/cold neutrons

- Wave-like nature and Bragg (elastic) scattering
- $\lambda = 2d\sin\theta$ - Same formalism as X-ray scattering
- powder diffractometers, sample geometry similar - just bigger

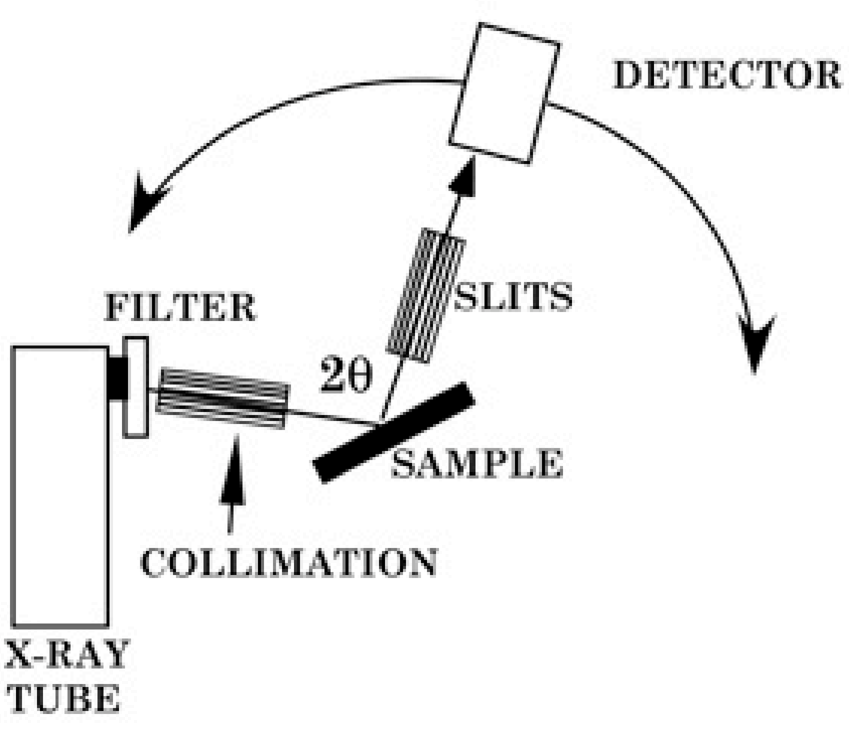


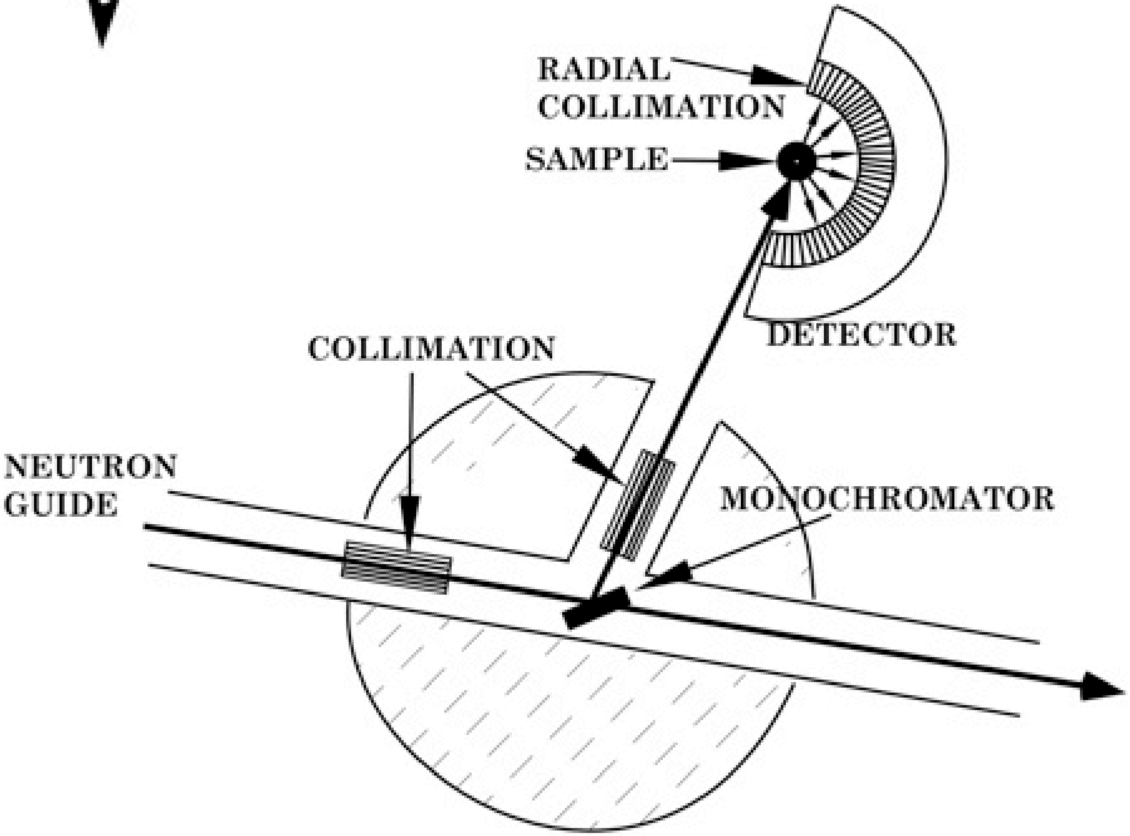
# powder diffractometers - just bigger



# powder diffractometers - just bigger

*Modern neutron powder diffractometers use multiple detector; neutrons come from weak sources (cf. X-ray synchrotrons)*





# Neutron intensities are low, so large detectors are needed

## Construction of a microstrip position-sensitive detector (printed circuit)

Anton Oed
Bruno Guerard
Pierre Convert
Thomas Hansen
Jacques
Torregrossa

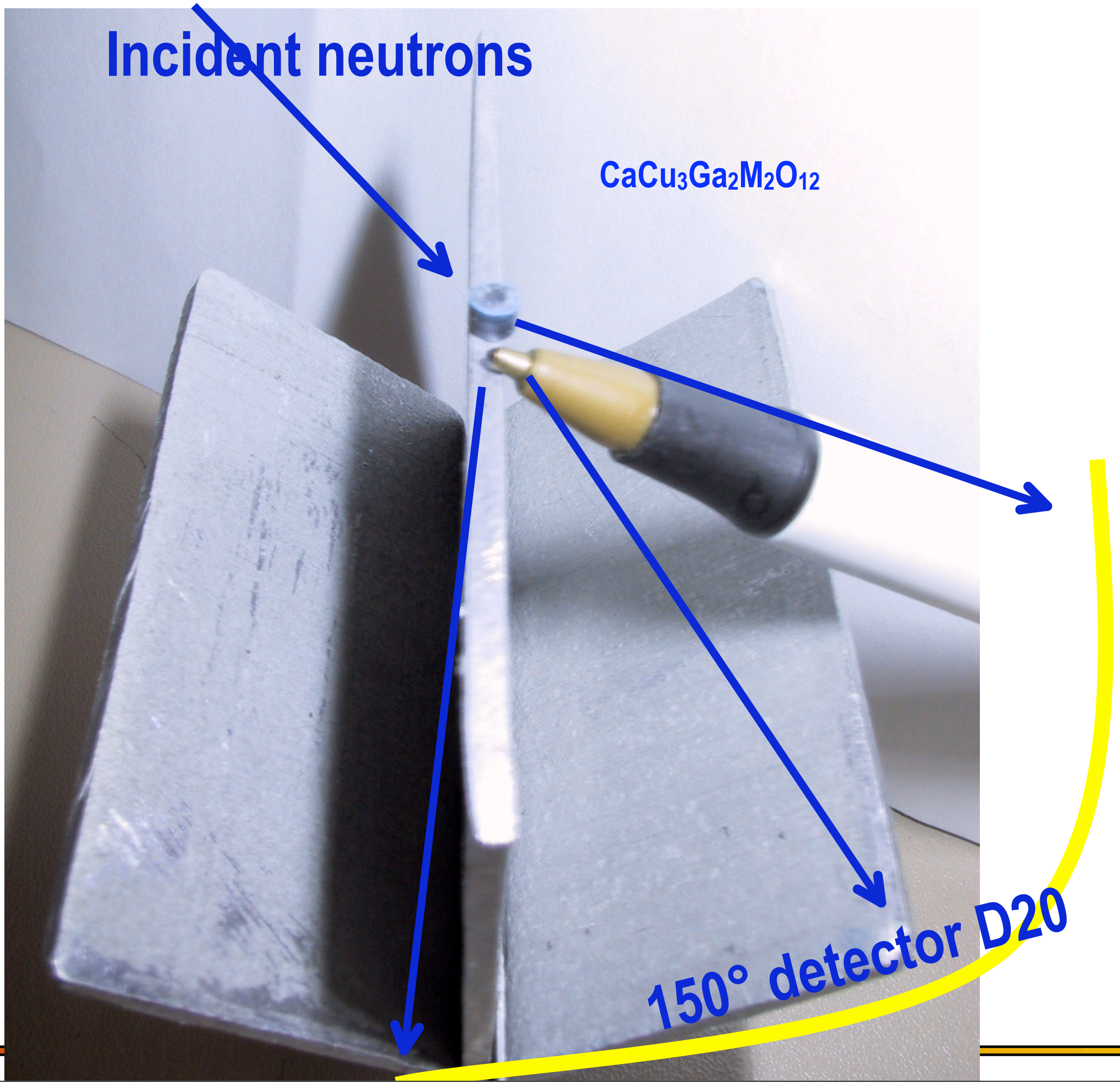
# Construction of a microstrip position-sensitive detector (printed circuit)

# Applications of large fast detectors/detector banks scattering

## Complete diffraction pattern in 20 min. on small samples - at ambient or in environmental (high P) cells

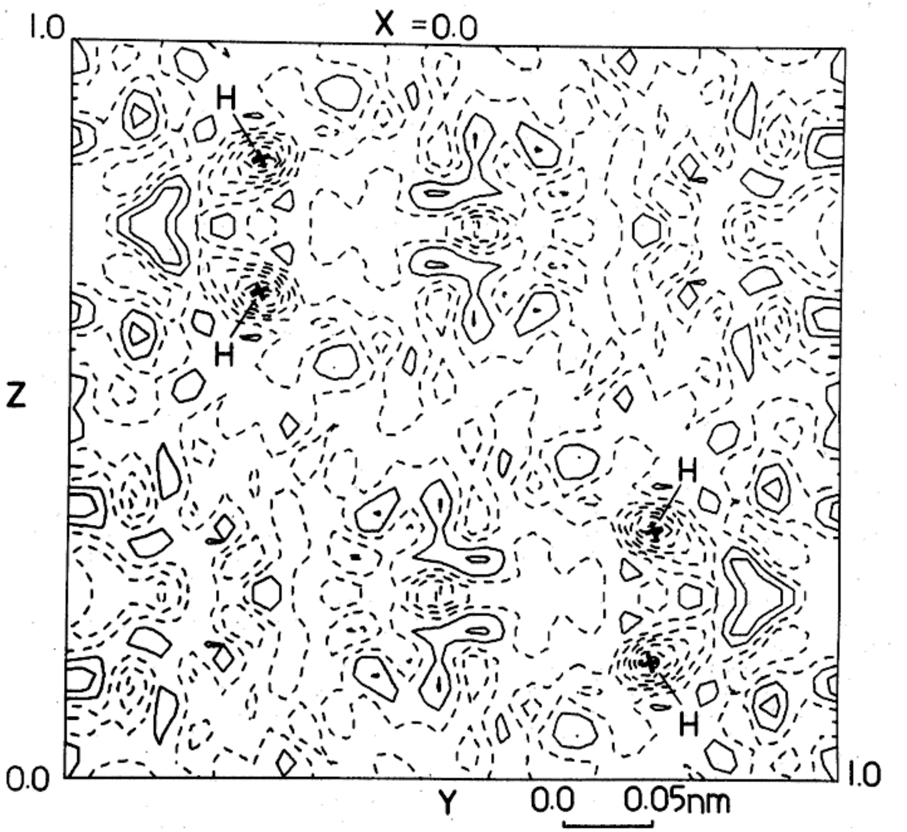
21 mm$^3$ pellet recovered from HP synthesis

Byeon,, Lufaso, Parise, Woodward, Hansen (2003) High-Pressure Synthesis and Characterization of Perovskites with simultaneous ordering of both the A- and B-site Cations, (M = Sb, Ta) Chem. Materials, 15, 3798-3804



# Light element sensitivity: finding H(D) in minerals

- Sites for H (or D) precisely determined
- H(D) in topaz and topaz-OH
- Even in small samples H-positions easily determined



1. Parise, Cuff, Moore (1980) Min Mag , 43, 943
2. Chen, Lager, Kunz et al. (2005) Acta Cryst., 61, 1253
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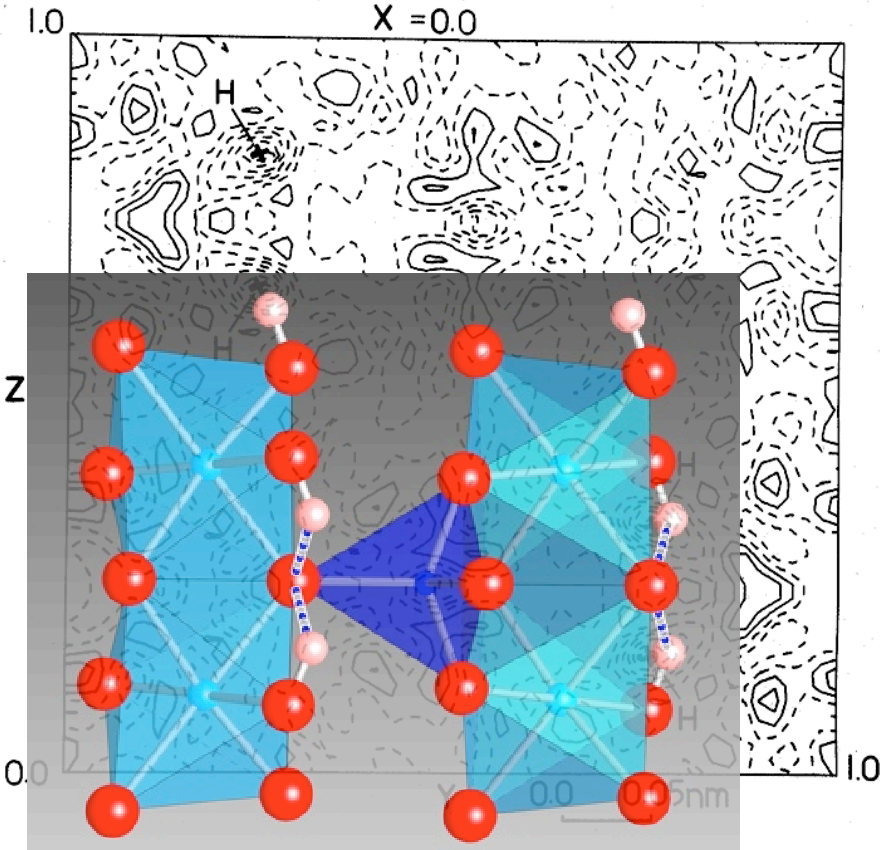

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# Light element sensitivity: finding H(D) in minerals

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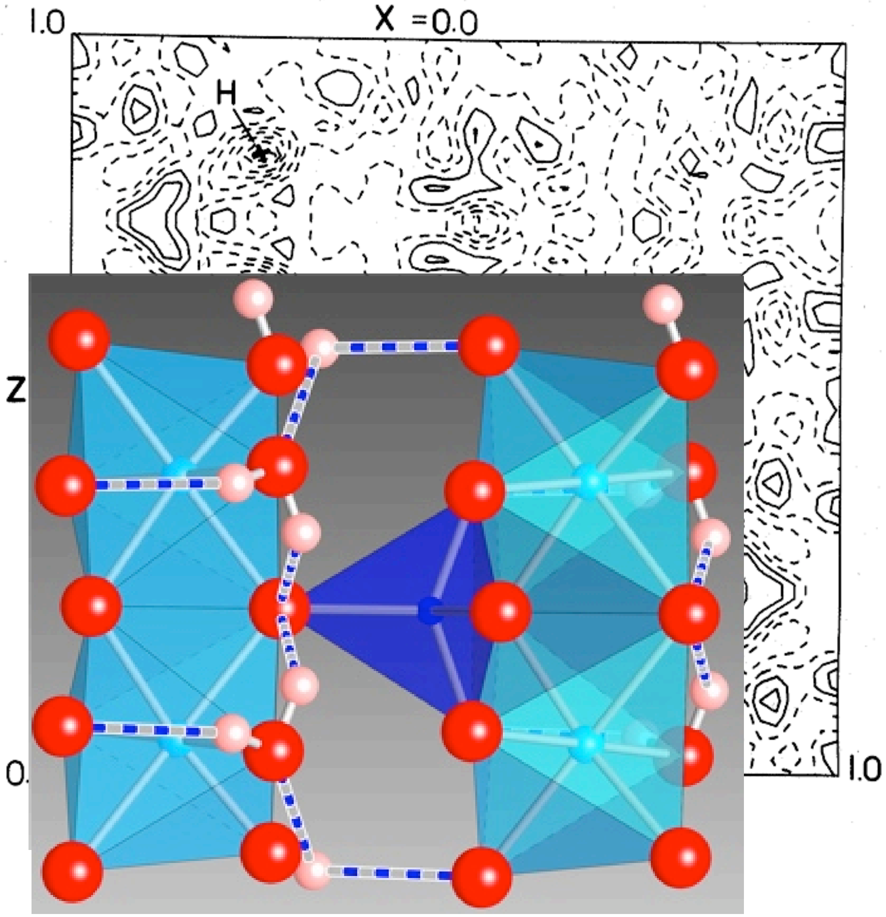
New positions revealed by recent ambient (2) and high pressure work (3)



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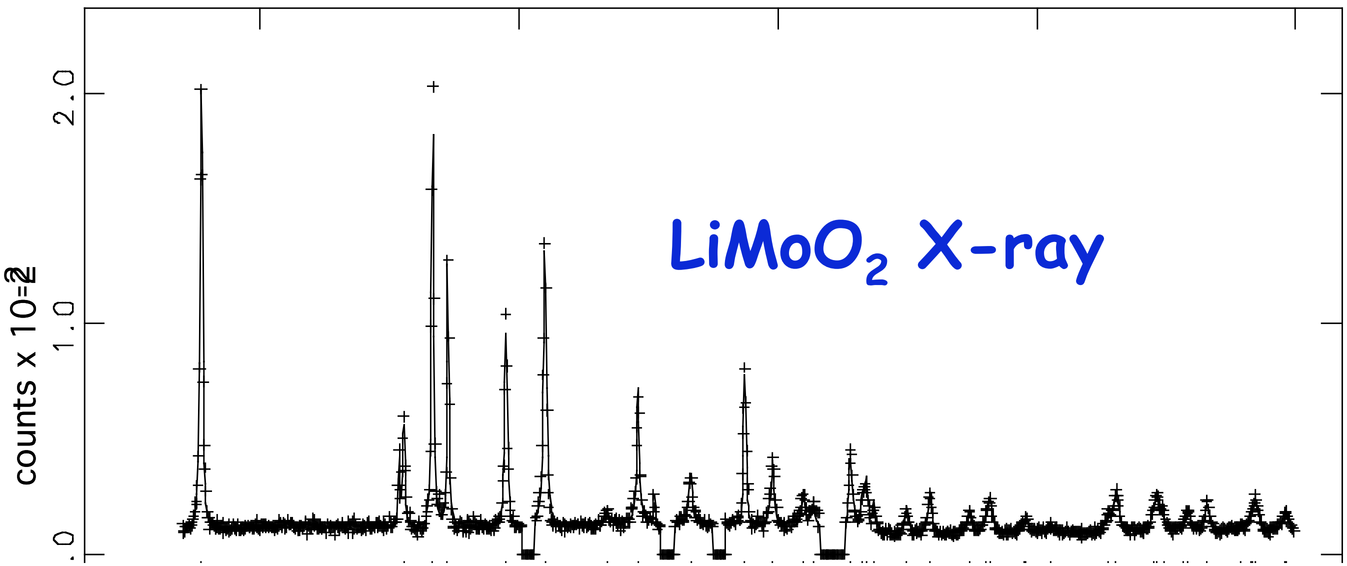
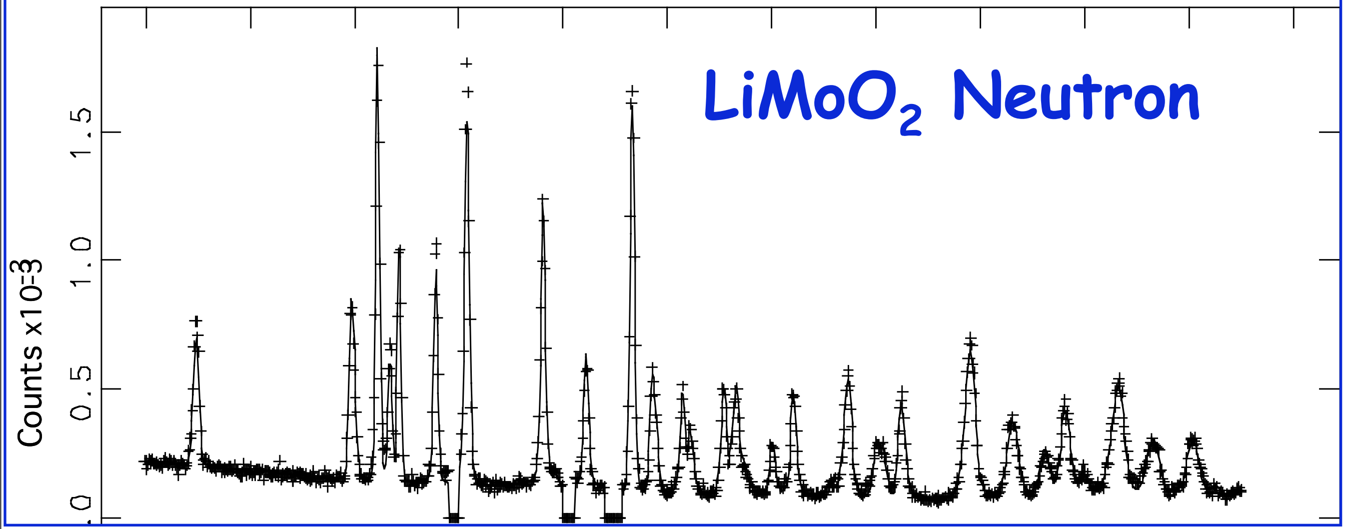
# Light element sensitivity: joint X-N structural refinements Note: less drop off in scattering at high angles for neutrons

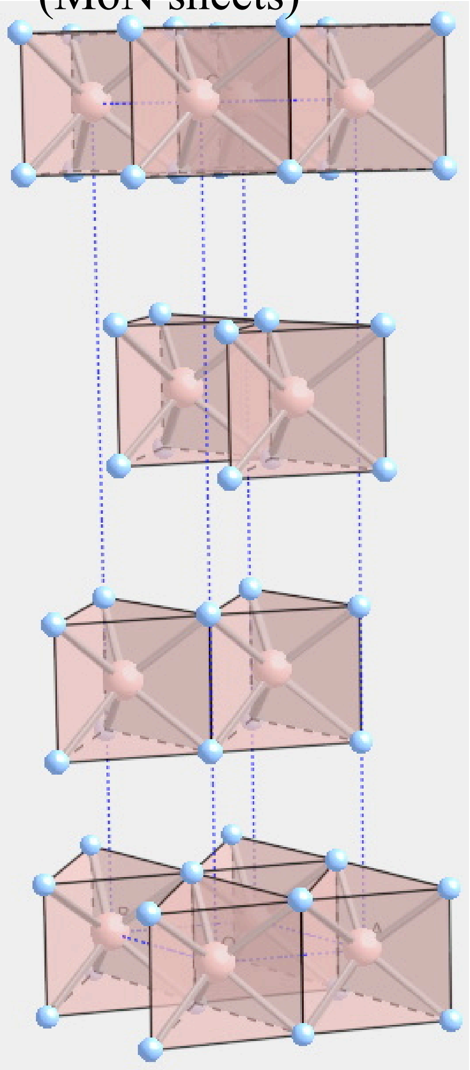
$LiMoN_2$ X-7A data capillary, Si(111), λ=0.7122Å, Ge(111) analyser, 1x7 mm slits, Kevex detector



$LiMoN_2$ H4S Vanadium tube, Si(111), λ=1.3585, graphite analyser, 20'-40'-40'-20' sollar slits



X-ray structure (MoN sheets)



Elder, Doerrer, DiSalvo, Parise, Duyomard, Tarascon, (1992) New Nitride - $LiMoN_2$. Chem. Mater. 4, 928

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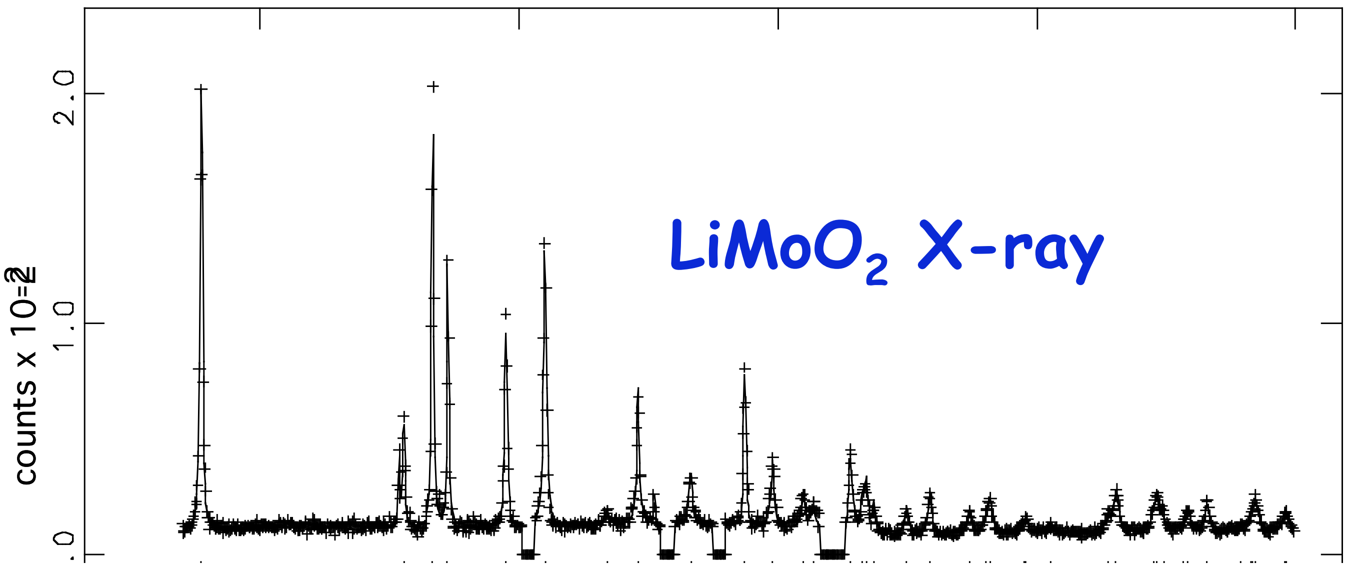

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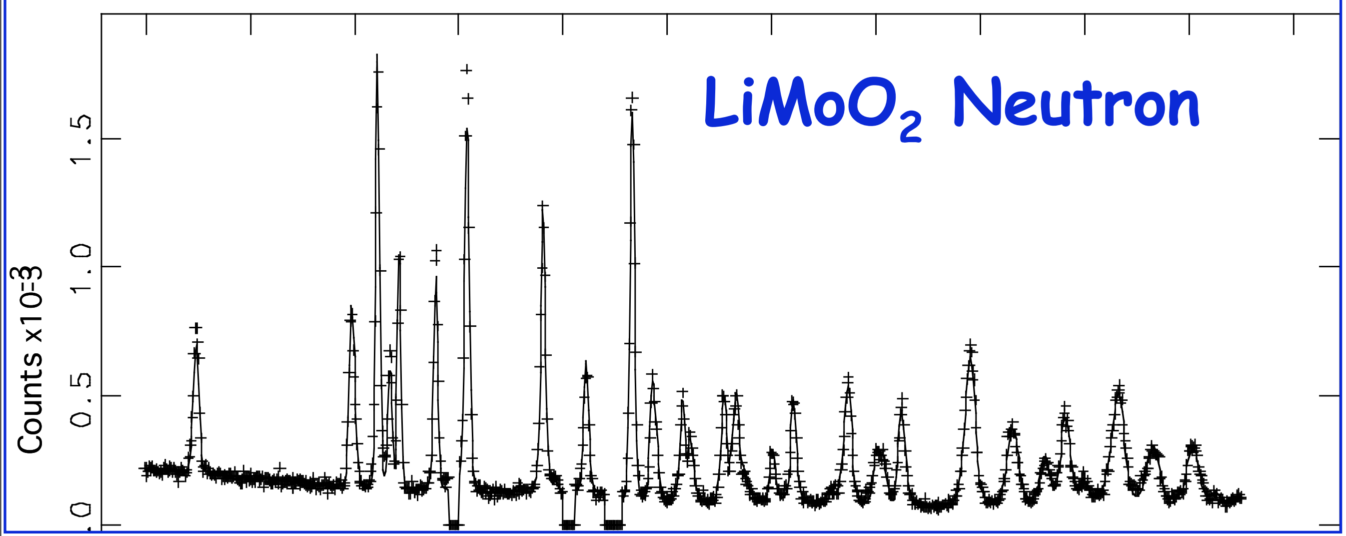
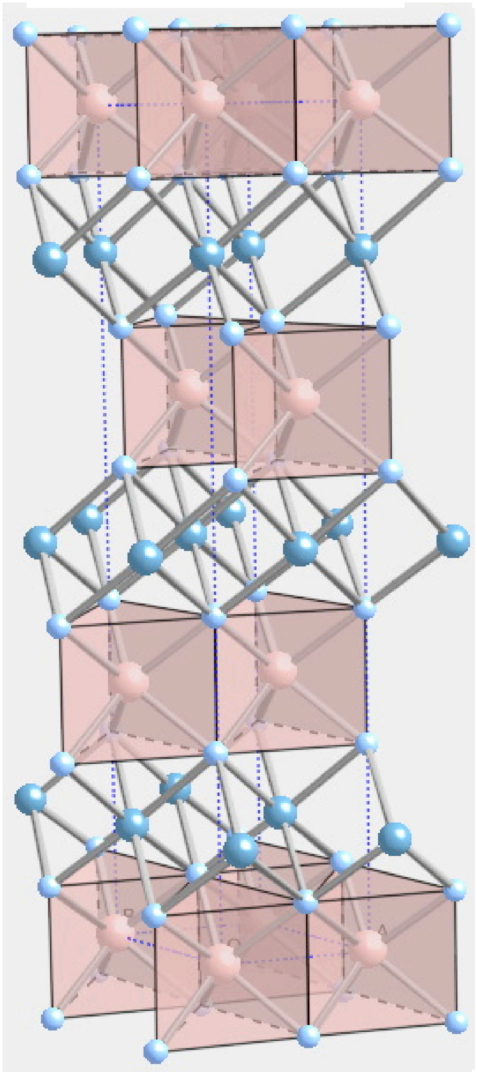


Li revealed in Neutron Structure



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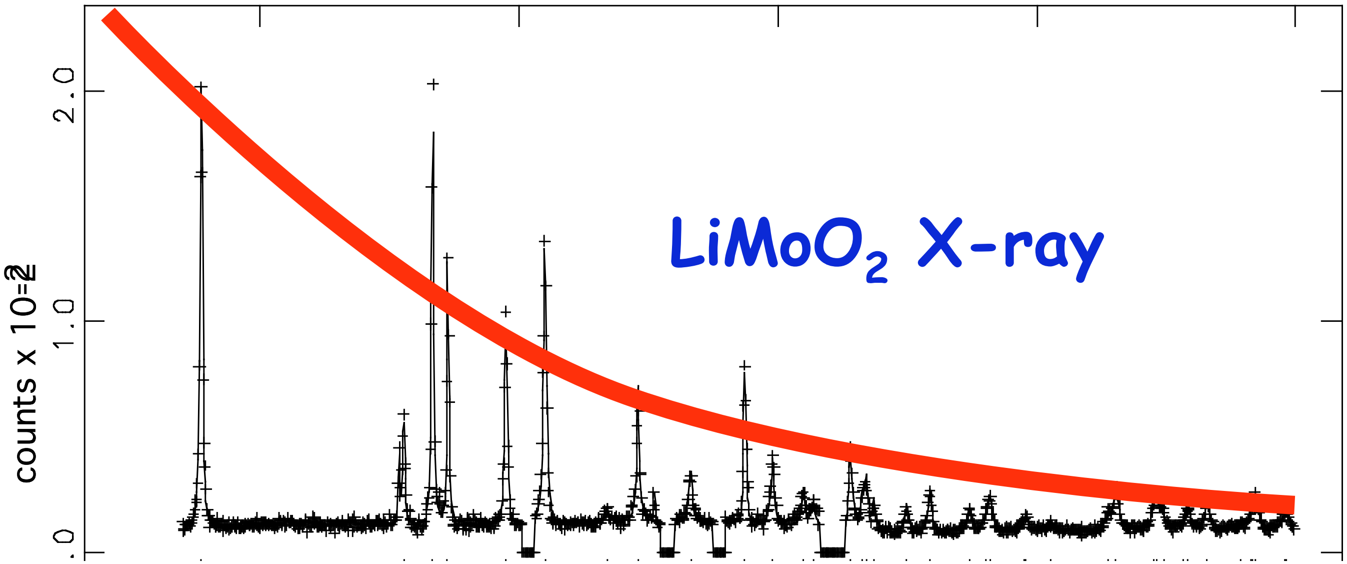

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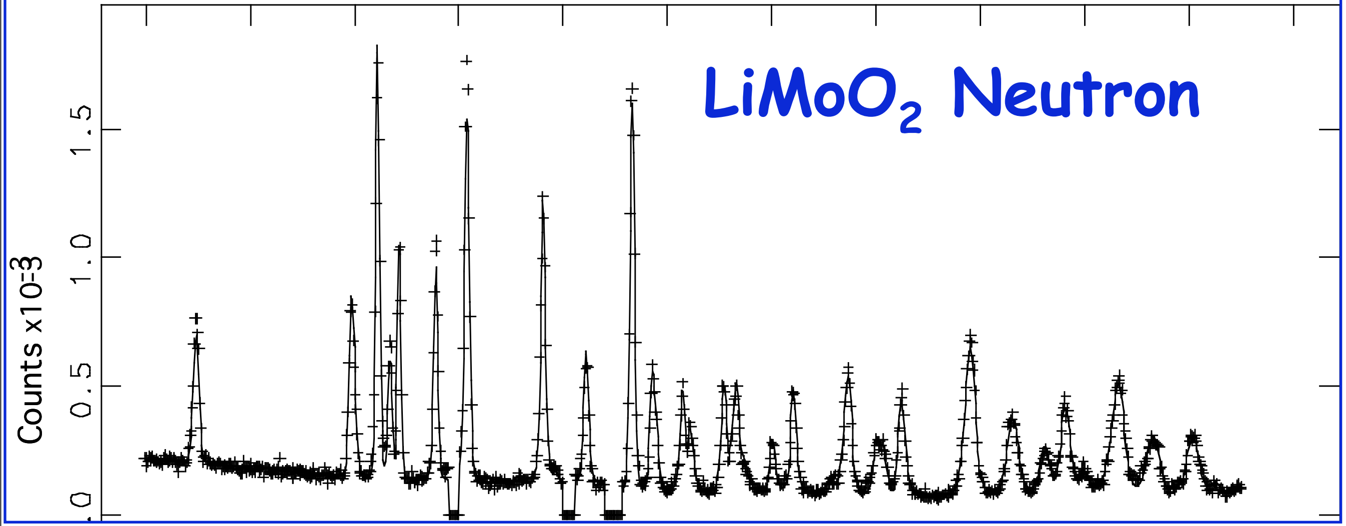

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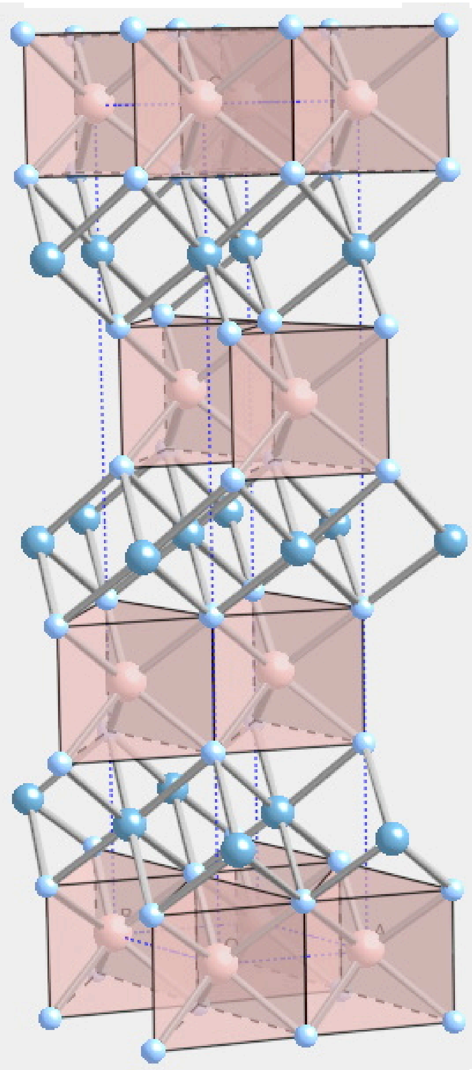

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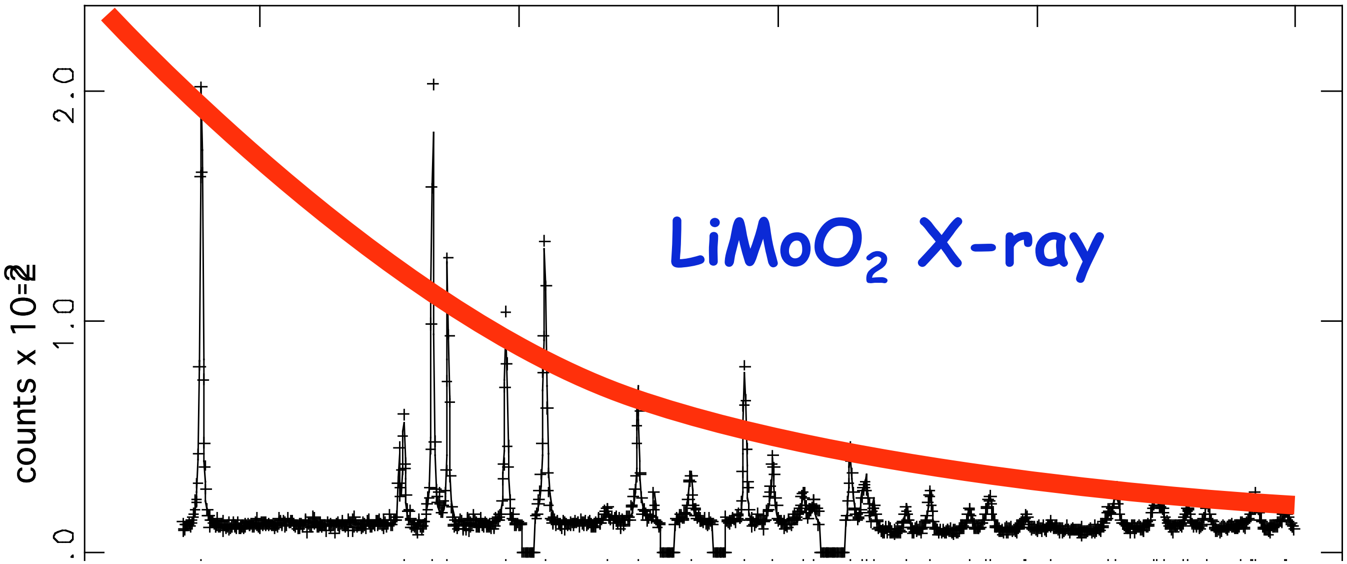

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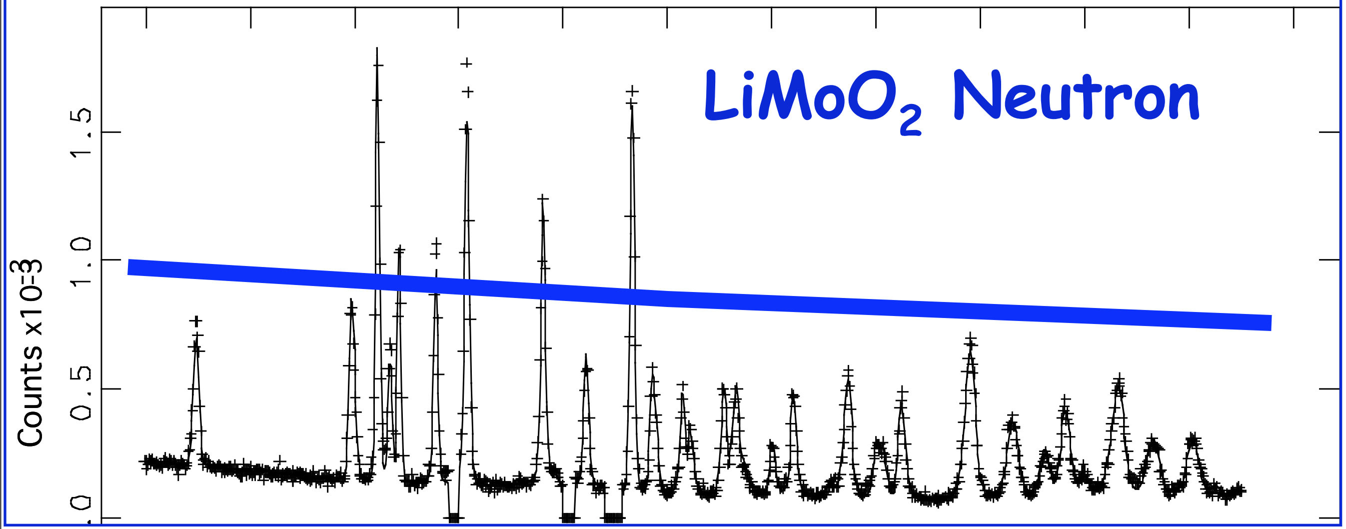

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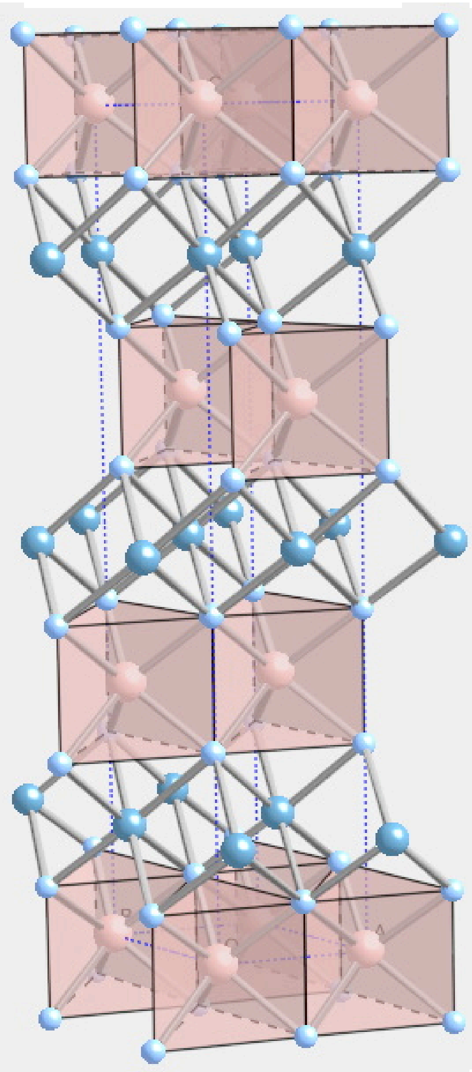

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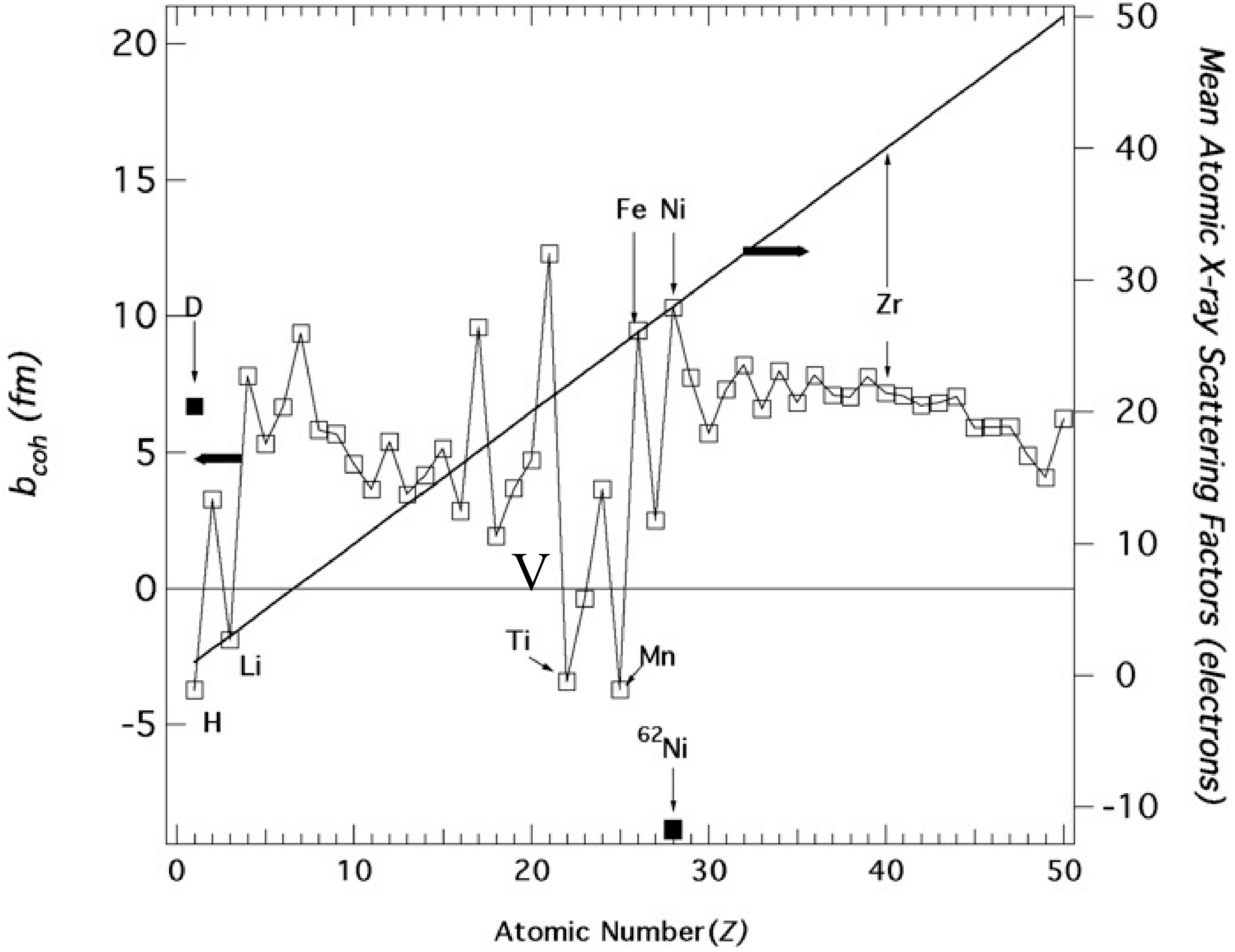
# Differences in scattering power for isotopes
# (2) Null scattering



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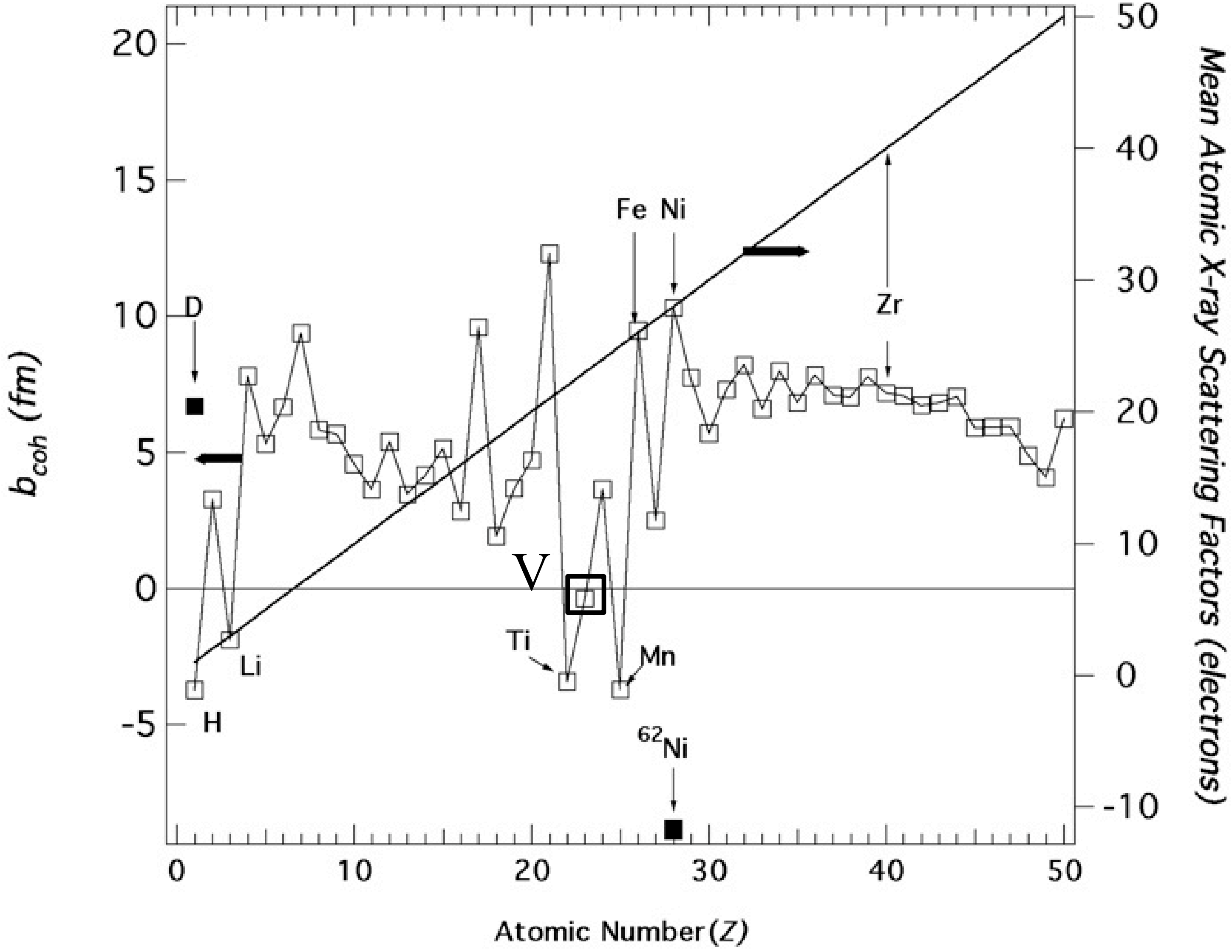

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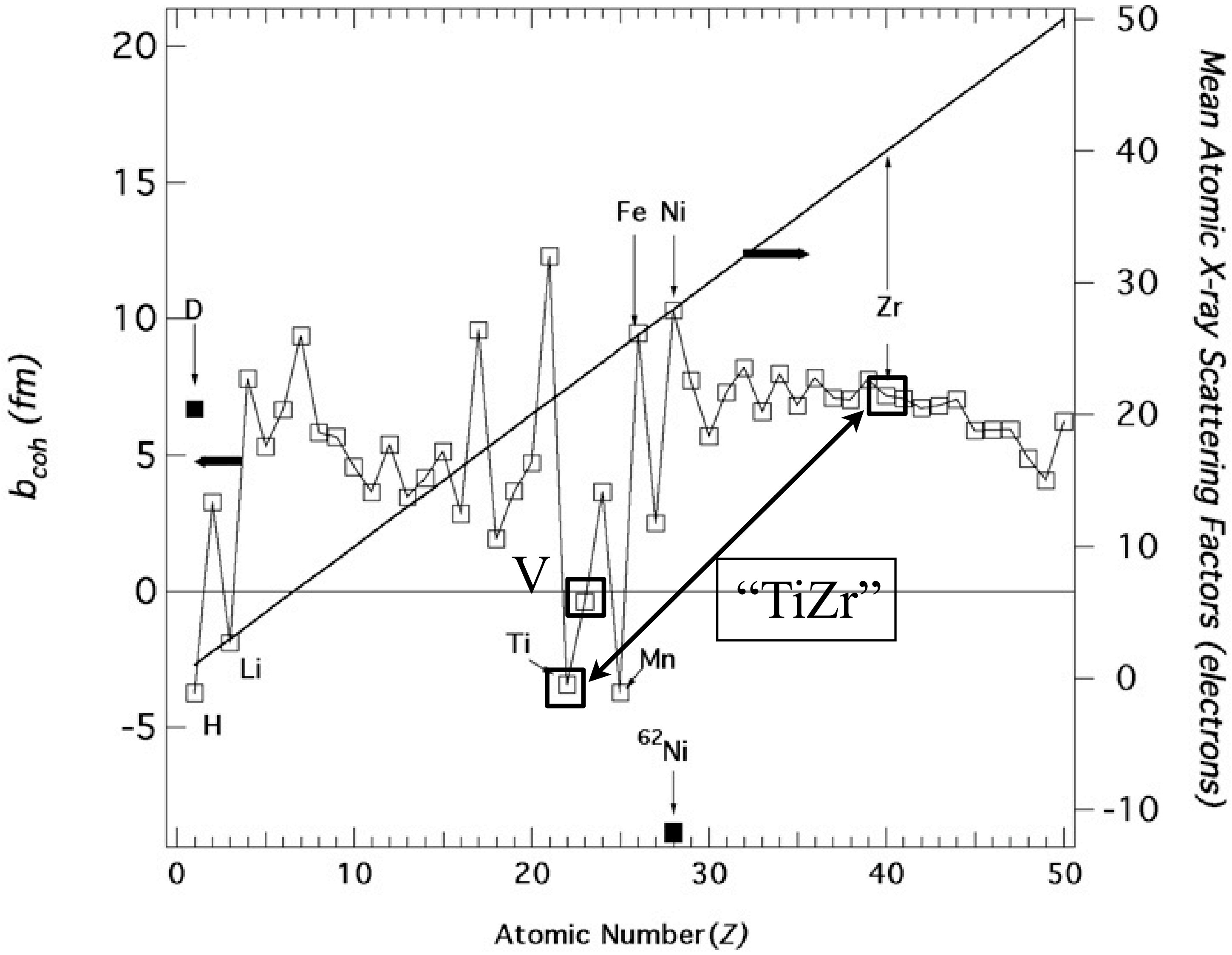

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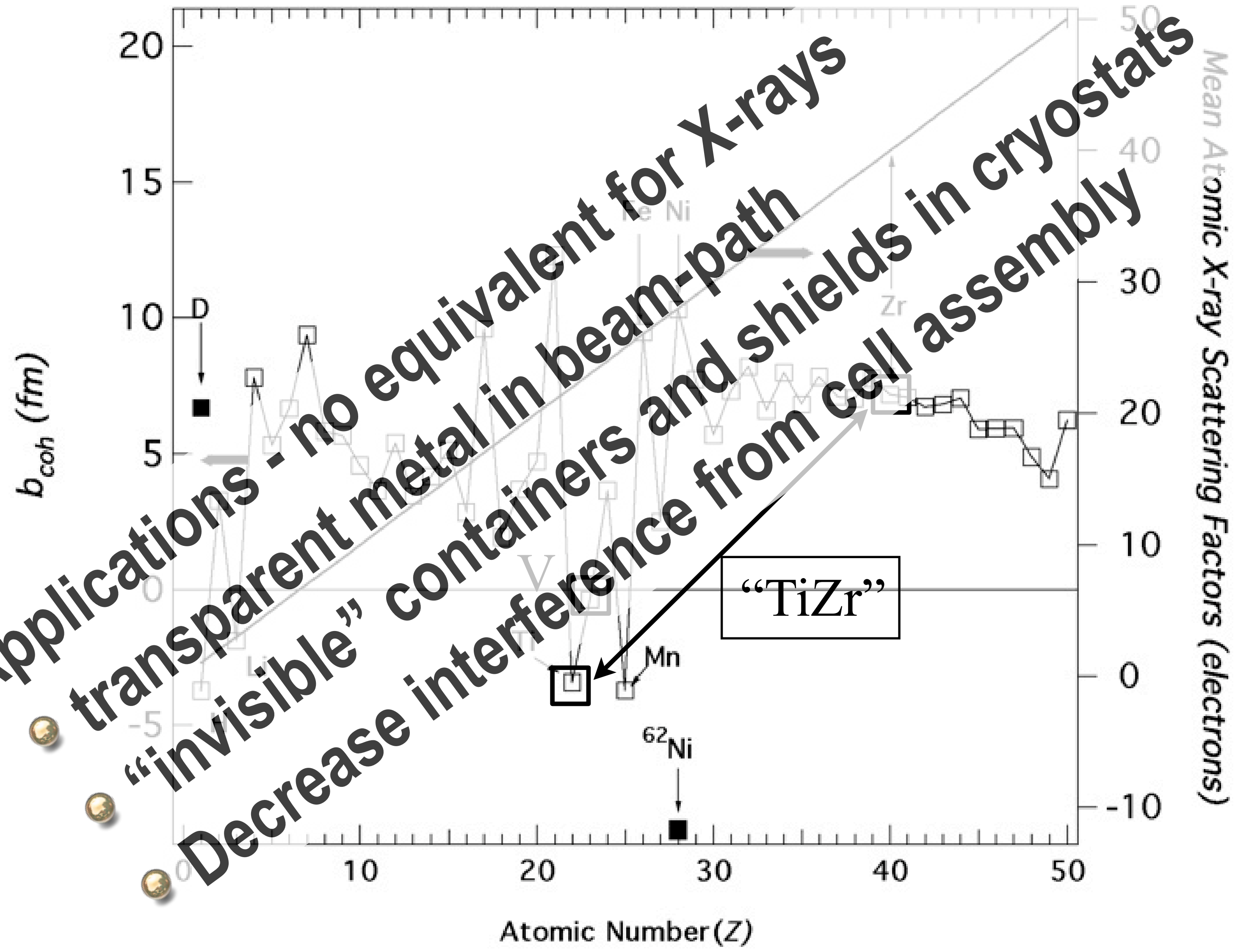
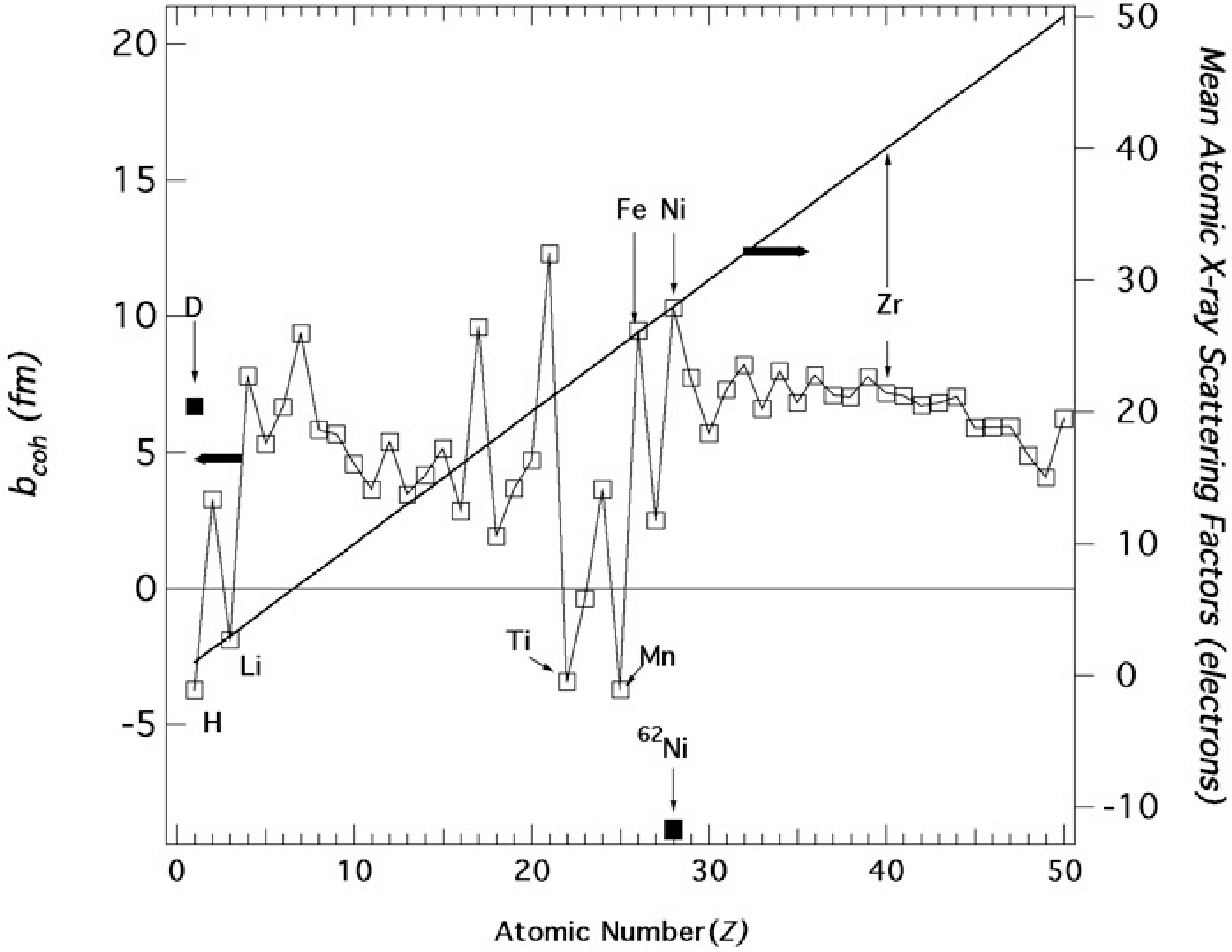


- Applications - no equivalent for X-rays
- transparent metal in beam-path
- "invisible" containers and shields in cryostats
- Decrease interference from cell assembly

# Differences in scattering power (3) Contrast variation



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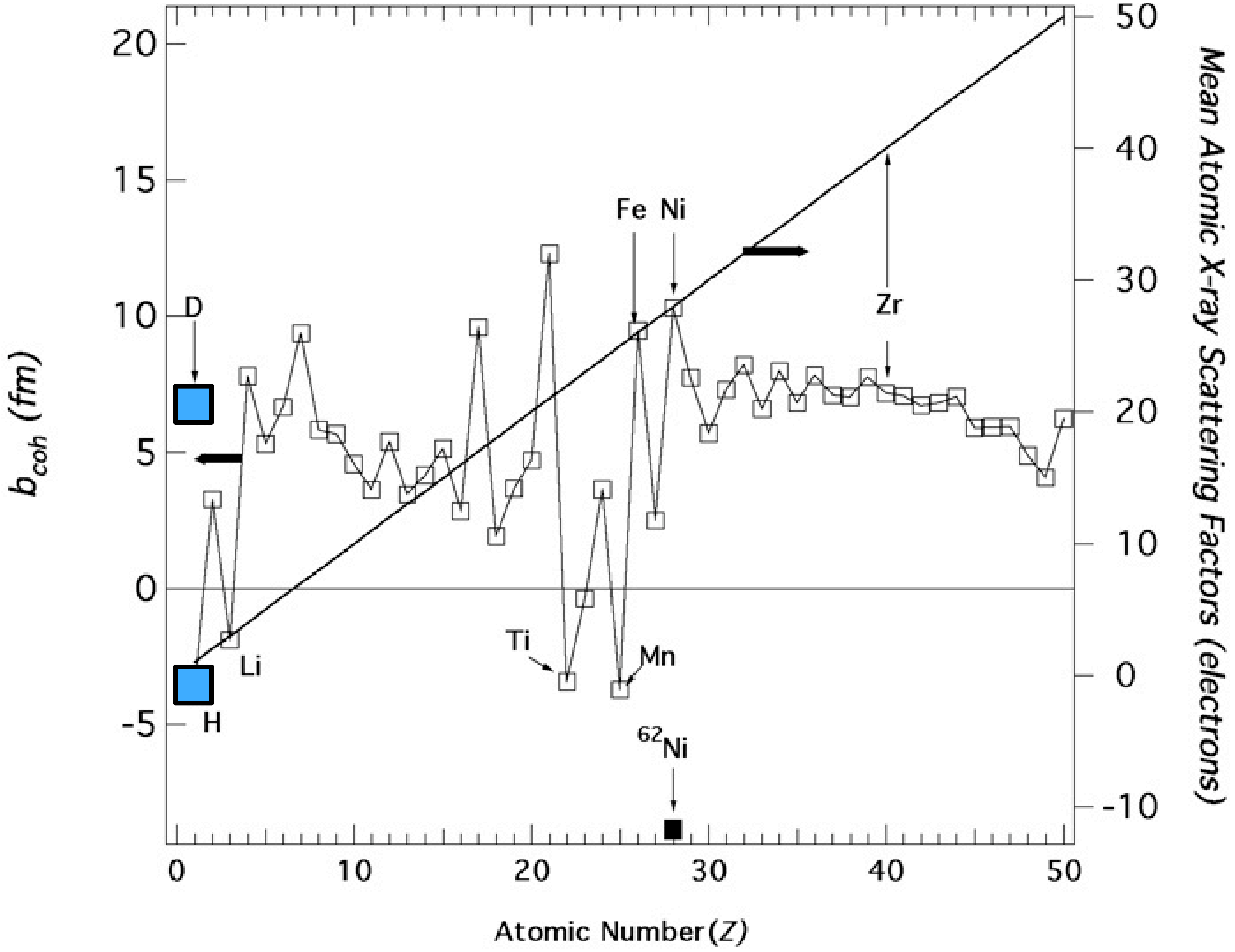

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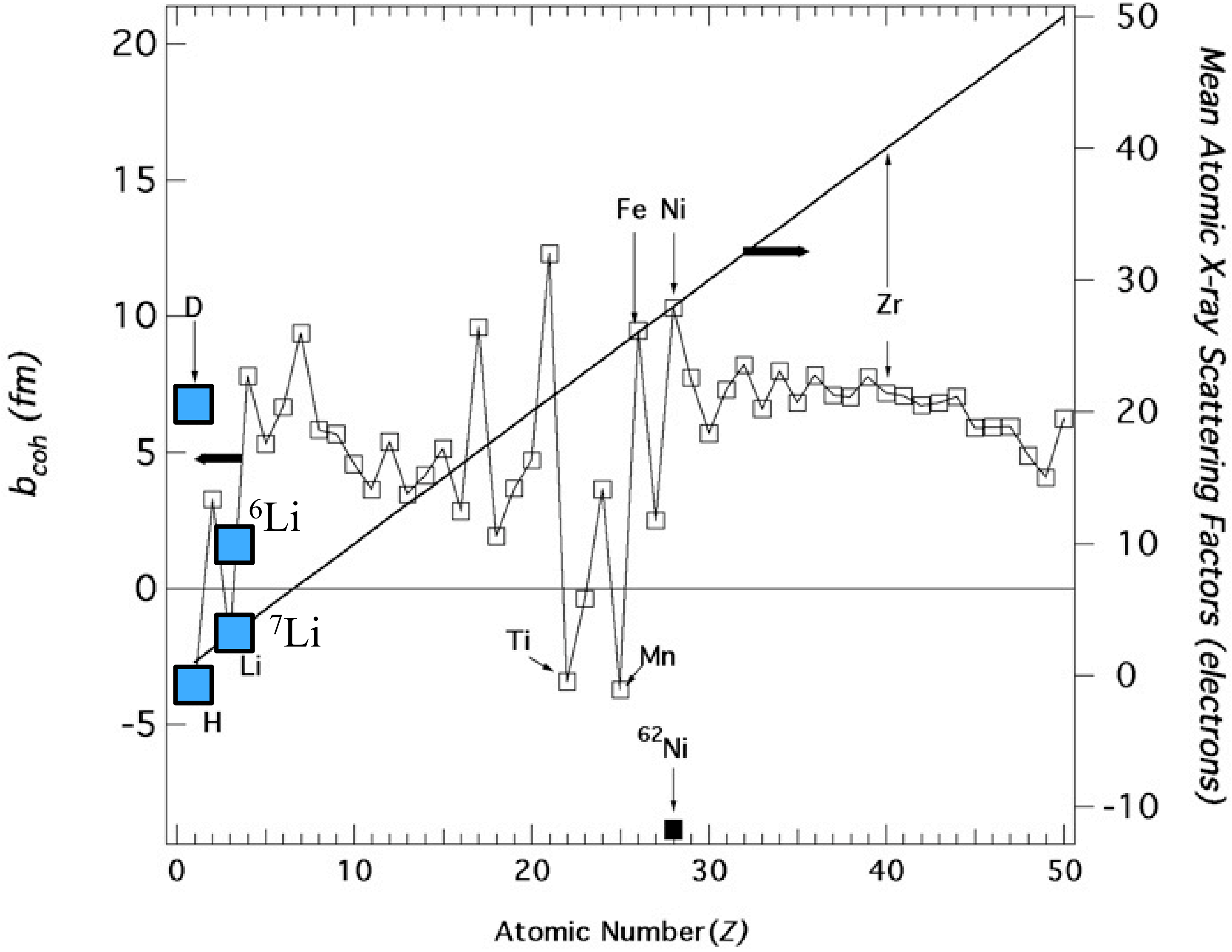

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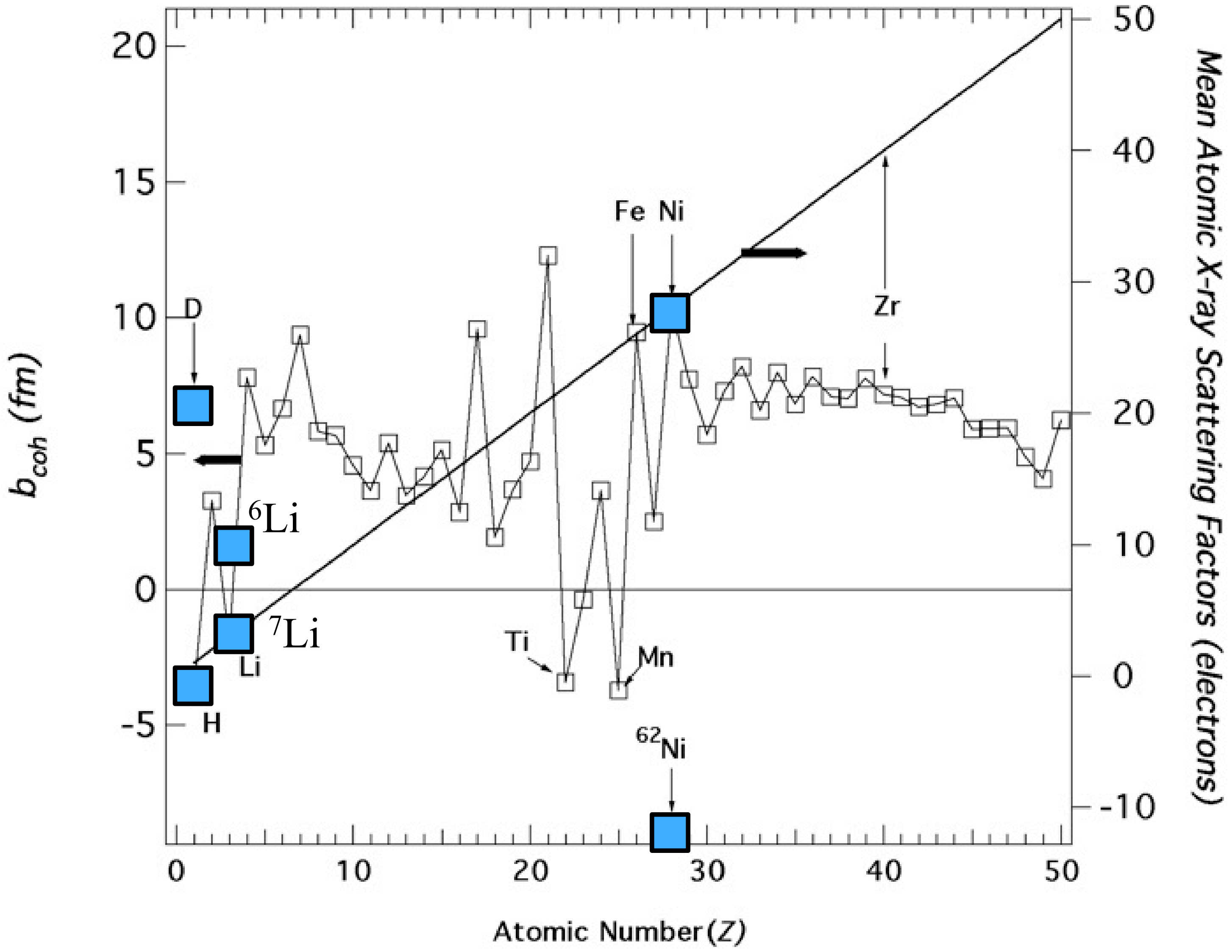
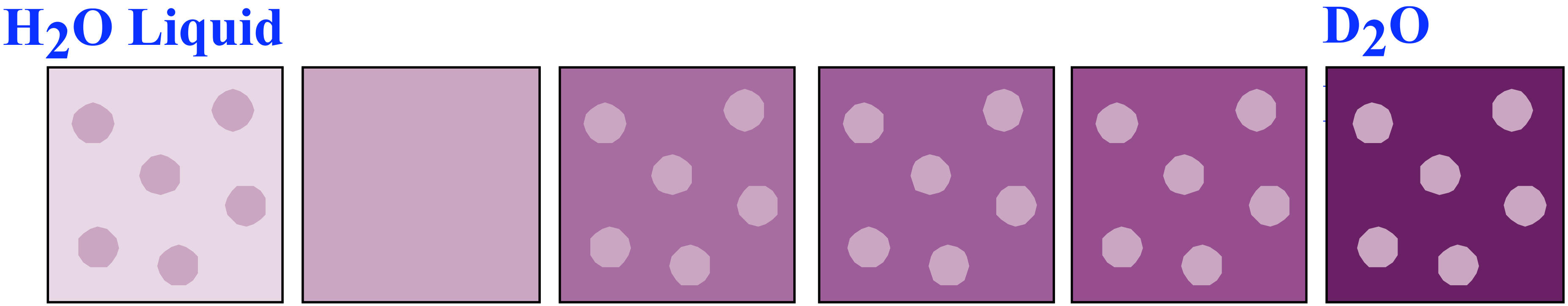


# Why Neutrons ?

- Neutrons are electrically neutral & more penetrating than X-rays.
  - tomography, radiography of real rocks and parts
- Neutrons act like particles
  - waveguides, gavitational effects
- Neutrons act like waves
    - Neutrons interact with nuclei & locate atoms more precisely.
      - Light atoms scatter neutrons as strongly as heavy atoms.
      - • $b_{coh}$ independent of Z, $\sin\theta/\lambda$, can be -ve
      - Diffraction, D/H contrast variation, precise positions, PDF
- Neutrons have a moment, & can determine magnetic structures.

- Neutrons can study atom dynamics & the forces between atoms.

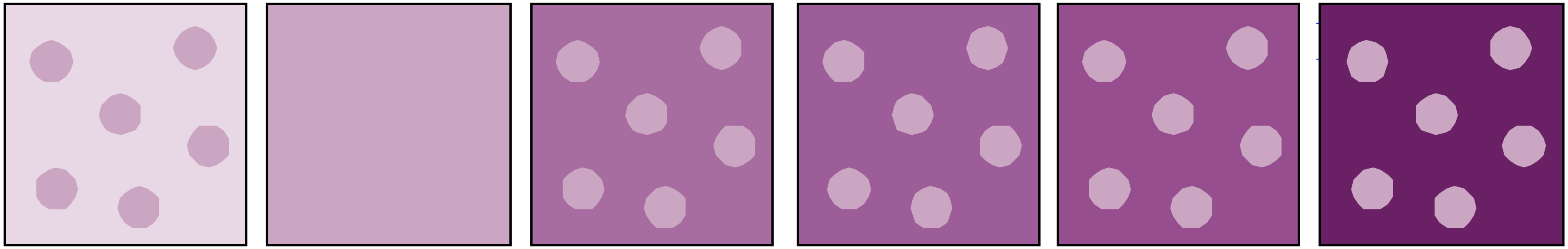
# Contrast variation: $b^{H}_{coherent}$ ~ -4 fm; $b^{D}$ ~ 6 fm; $b^{O}$~ 5 fm; $b^{H2O}$~ -3 fm, $b^{D2O}$~ 17 fm



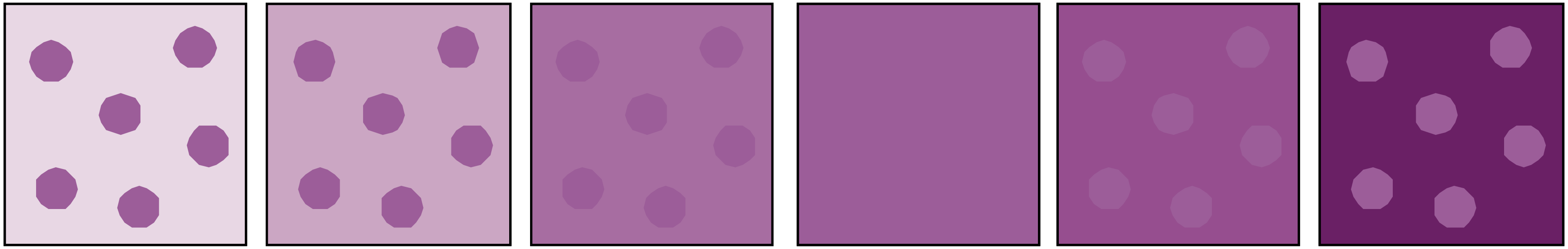
Hydrogenous particles

# Contrast variation: $b^{H}_{coherent} \sim -4$ fm; $b^{D} \sim 6$ fm; $b^{O} \sim 5$ fm; $b^{H_2O} \sim -3$ fm, $b^{D_2O} \sim 17$ fm

**$H_2O$ Liquid** **$D_2O$**



**Hydrogenous particles**



**Less Hydrogenous particles**

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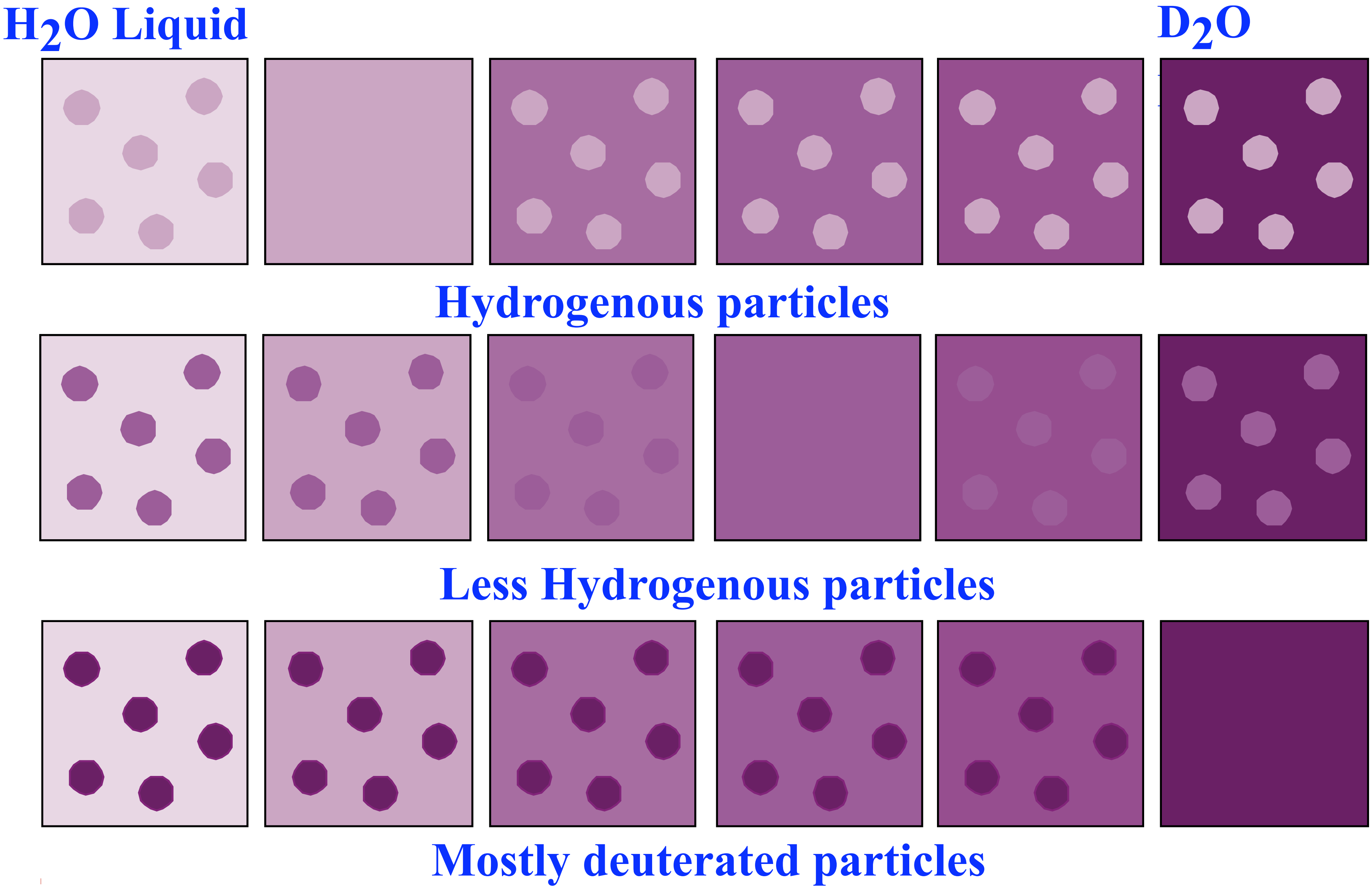

**$H_2O$ Liquid**

**$D_2O$**

**Hydrogenous particles**

**Less Hydrogenous particles**

**Mostly deuterated particles**

# Differences in scattering power (3) Contrast variation

- Applications
  - Deriving partial G(r) by choosing appropriate isotopes

***$LiNi_{0.5}Mn_{0.5}O_2$ - site disorder of ALL metals over sites (Not HP)***

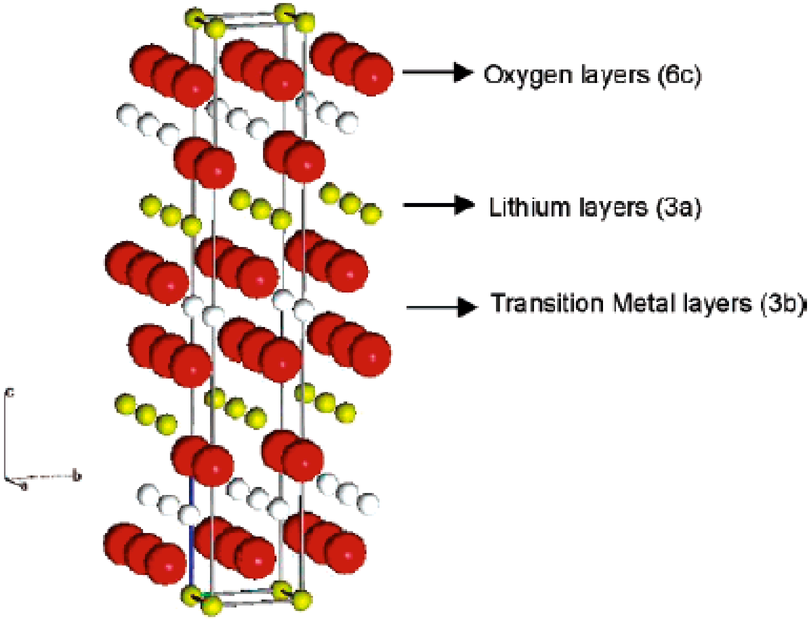

**Figure 1.** Ideal structural model of $LiNi_{0.5}Mn_{0.5}O_2$ based on $LiCoO_2$ (α-$NaFeO_2$ structure, space group $R\bar{3}m$, $a = b = 2.8874$ Å, $c = 14.2825$ Å,

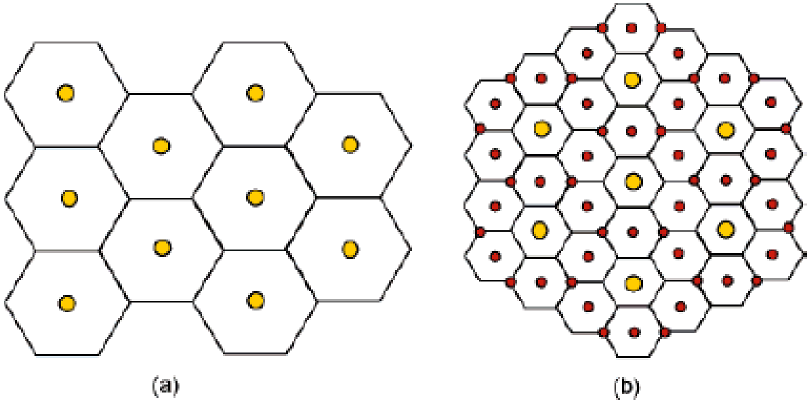

**Figure 2.** (a) A view of the honeycomb ordering found in the *ab* planes of $Li_2MnO_3$ along the *c*-axis. Each Li atom (in yellow) in the Li/Mn layers

Breger, Dupre, Chupas,Lee, Proffen, Parise, Grey (2005), JACS, 127, 7529

# Differences in scattering power (3) Contrast variation

- Applications
  - Deriving partial G(r) by choosing appropriate isotopes

$$G(r) = 4\pi r[\rho(r) - \rho_0] = \frac{2}{\pi}\int_0^{\infty} Q[S(Q) - 1]\sin(Qr)dQ$$

***Determined experimentally (note this is G(r) not g(r) and its neutrons - it can be negative)***

$$G_c(r) = \frac{1}{r}\sum_i\sum_j\left[\frac{b_i b_j}{\langle b\rangle^2}\delta(r - r_{ij})\right] - 4\pi r\rho_0$$

***Determined from model***

***Breger, Dupre, Chupas,Lee,Proffen,Parise,Grey (2005), JACS, 127, 7529***

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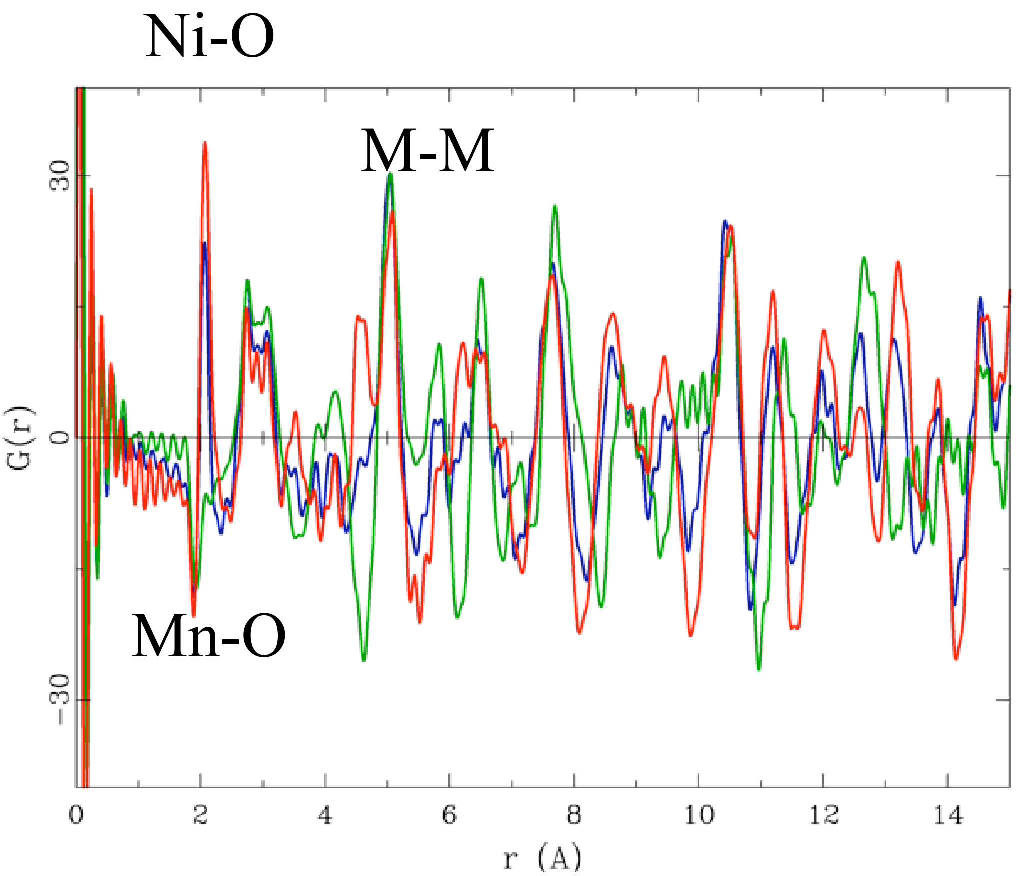
***Determined from model***

***Now, if $b_i$ and/or $b_j$ is zero, the partial (contributions from atom pair involving i), disappears. How do we play this game?***

*Breger, Dupre, Chupas,Lee,Proffen,Parise,Grey (2005), JACS, 127, 7529*

# Differences in scattering power (3) Contrast variation

- **Applications**
  - **Deriving partial G(r) by choosing appropriate isotopes**



$G(r)$ of

$^7LiNi_{0.5}Mn_{0.5}O_2$ (blue)

$^7Li^{ZERO}Ni_{0.5}Mn_{0.5}O_2$ (green)

$^6LiNi_{0.5}Mn_{0.5}O_2$ (red)

$b_{Li\text{-}6} = 2; \quad b_{Li\text{-}7} = -2$
$b_{Ni\text{-}58} = 14; \ b_{Ni\text{-}62} = -9$
$b_{Mn} = -4$

***Breger, Dupre, Chupas,Lee,Proffen,Parise,Grey (2005), JACS, 127, 7529***

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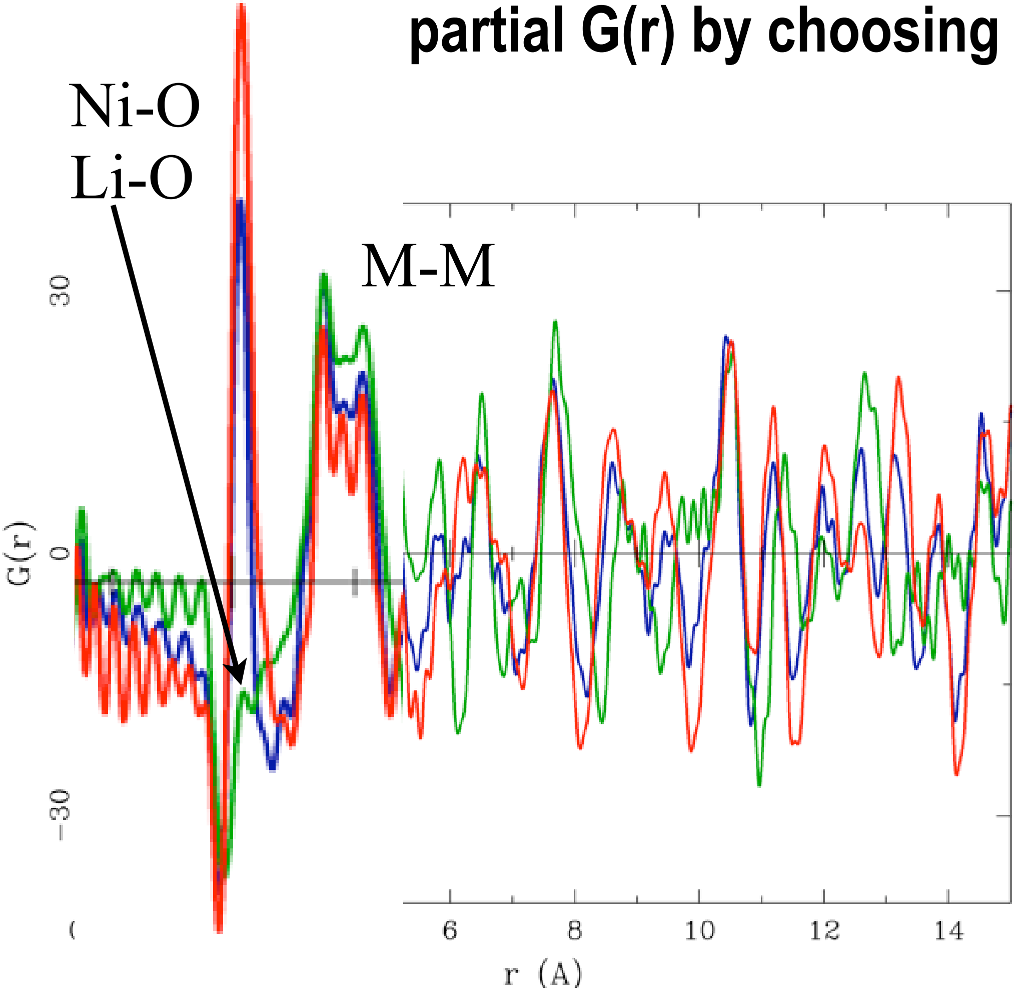

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# X-ray scattering vs. neutron scattering

## SUMMARY

- *X-rays scattered by electrons*
- *Cross-section increases with # of electrons*
- *Cross-section decreases with Q* $[Q=4\pi\sin\theta/\lambda]$
- *Energy: 5,000 eV to 100,000 eV*

- *Neutrons scattered by nucleus*
- *Cross-sections “random” (function of isotope)*
- *Cross-section independent of Q*
- *Energy: 0.001 eV to 0.2 eV*

# X-ray scattering vs.  neutron scattering

## SUMMARY

**More penetrating; larger samples needed.**

**Good for light elements (usually).**

**Good high “angle” data -- provides more accuracy**

**Right range for diffusion & atom vibrations (BIGGER % change upon interaction)**

- *Neutrons scattered by nucleus*
- *Cross-sections “random” (function of isotope)*
- *Cross-section independent of Q*
- *Energy:  0.001 eV to 0.2 eV*

# Types of neutron scattering phenomena

| | *Elastic Scattering* | *Inelastic Scattering* |
|---|---|---|
| *Coherent Scattering* | | |
| *Incoherent Scattering* | | |

**Much of the impact of neutron scattering related to inelastic - especially phonons and spectroscopic studies**

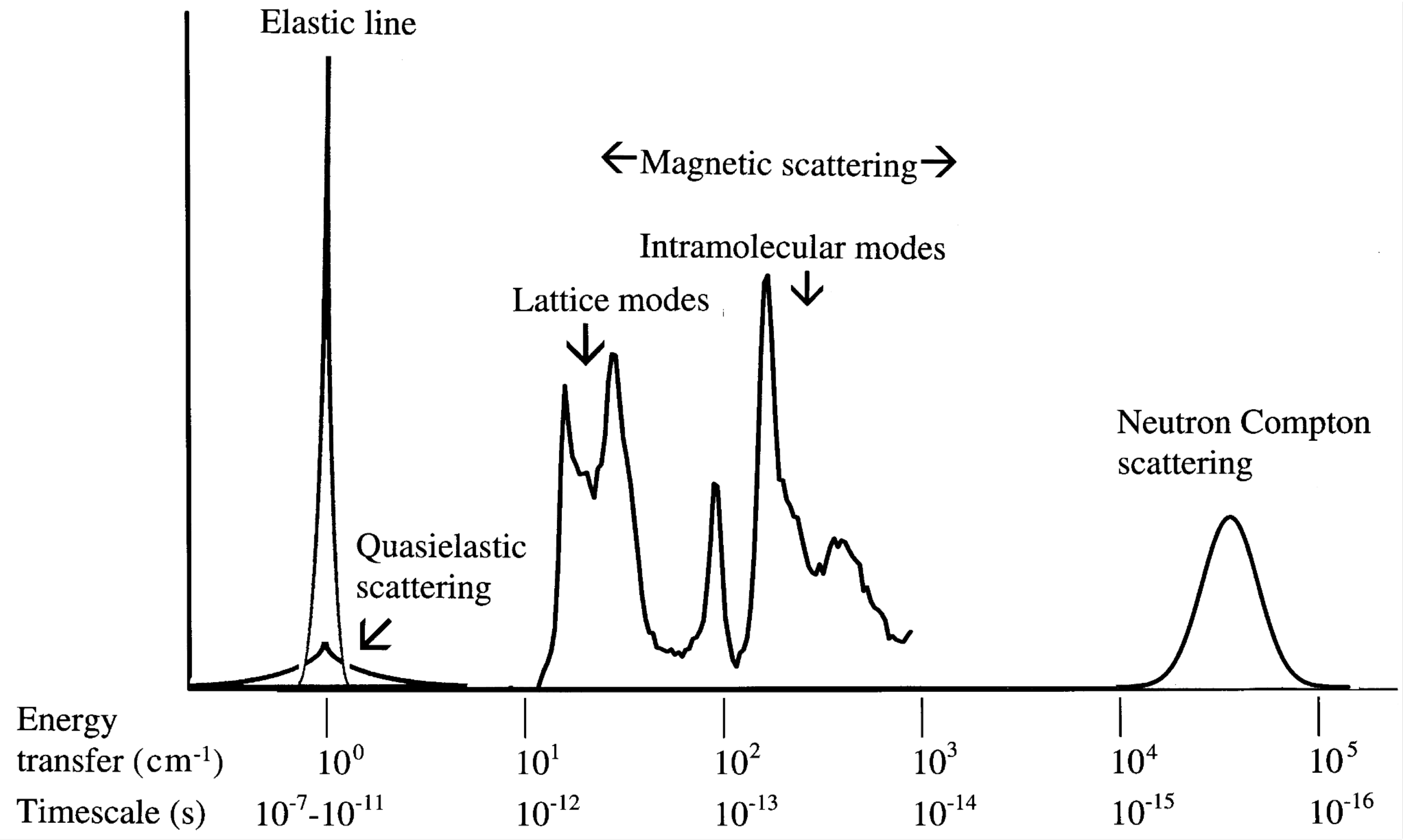
# Types of neutron scattering phenomena

| | *Elastic Scattering* | *Inelastic Scattering* |
|---|---|---|
| *Coherent Scattering* | Diffraction<br>(structural studies) | Phonons, magnons…<br>(collective excitations)<br>periodic and interference effects |
| *Incoherent Scattering* | QENS<br>(diffusion, low barrier motion) | Neutron Spectroscopies<br>(atomic vibrations) |

**Much of the impact of neutron scattering related to inelastic - especially phonons and spectroscopic studies**

# Inelastic neutron scattering?

Addresses questions of the directions and time-dependence of atomic motions.
periodic, correlated or uncorrelated (diffusion for eg)?
Etc.



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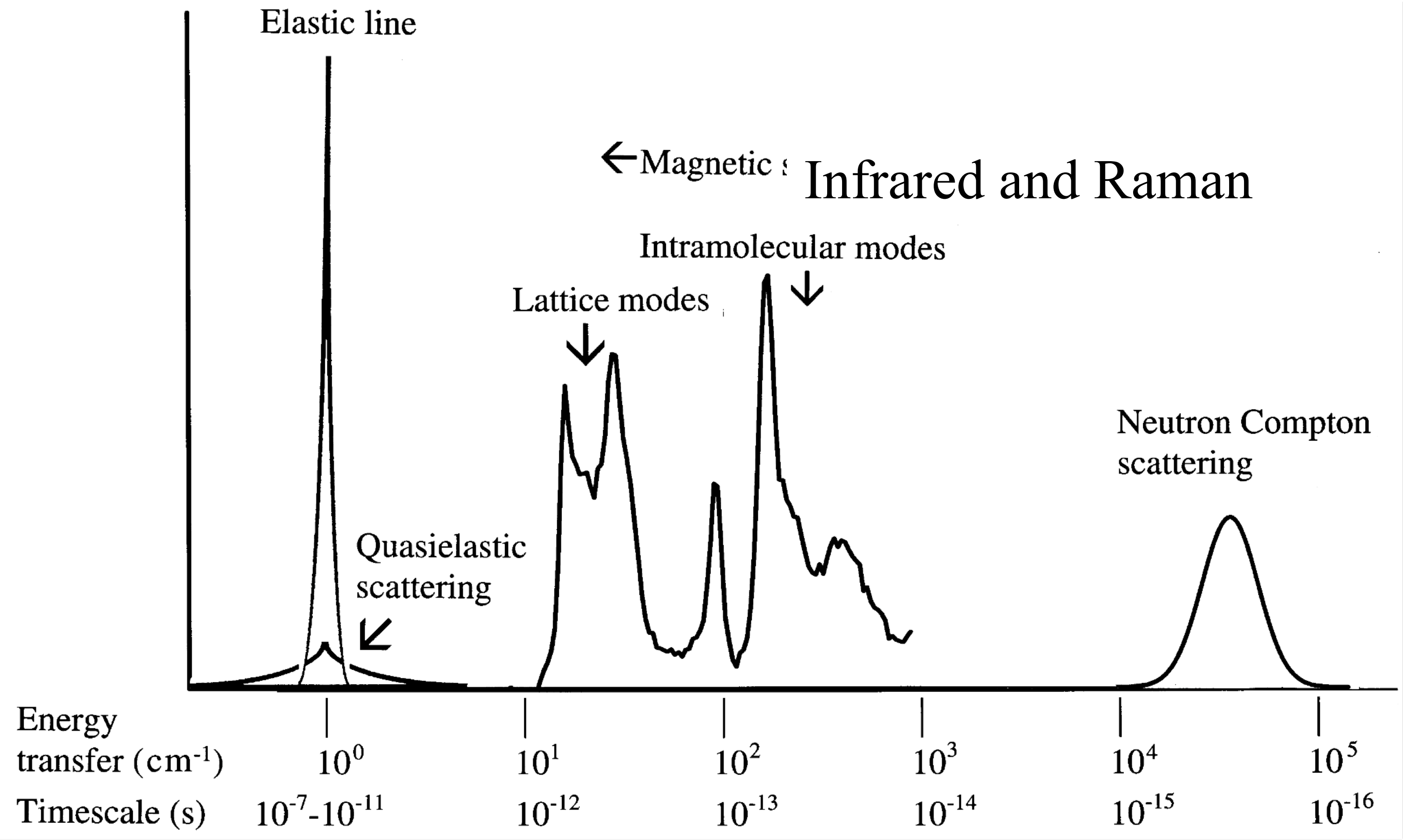
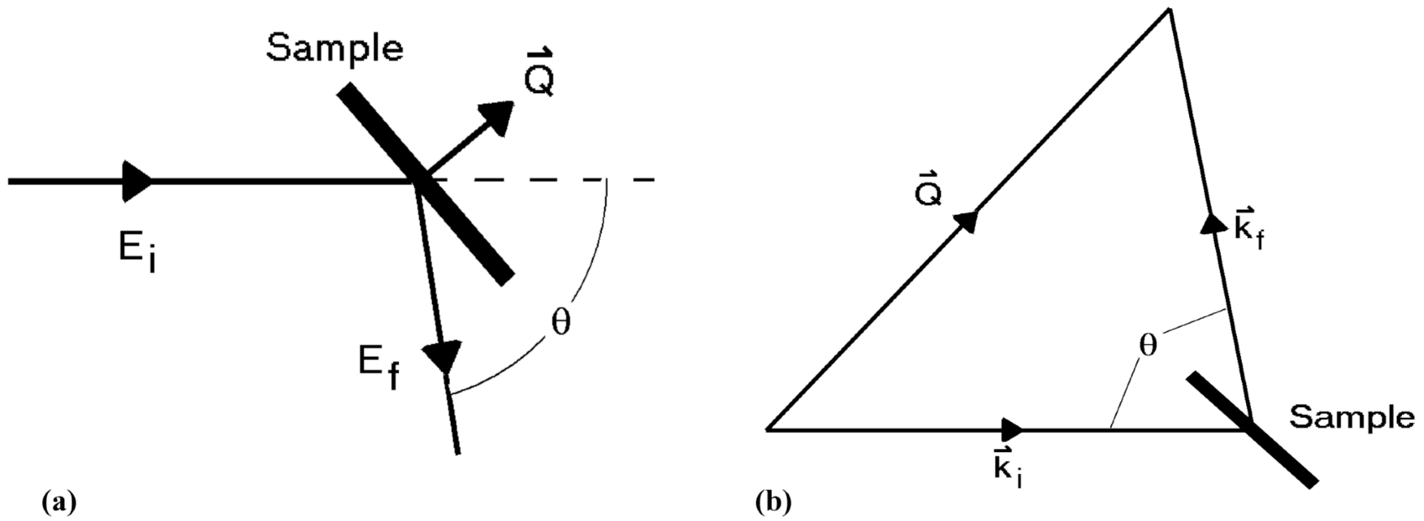


# Inelastic scattering in Real & Reciprocal space

**The neutron changes both energy and momentum when inelastically scattered by moving nuclei**



$$E_T = E_i - E_f \qquad Q = ki - k_f$$

**These equations define the accessible energy and momentum transfers: limit of energy transfer = neutron energy and momentum is conserved; this is a huge range and covers wide variety of phenomena**

# Expressions for $S(Q,\omega)$ can be worked out for e.g.

- Excitation or absorption of one quantum of lattice vibrational energy (phonon)
- Various models for atomic motions in liquids and glasses
- Various models of atomic & molecular translational & rotational diffusion
- Rotational tunneling of molecules
- Magnons and other magnetic excitations such as spinons
- Inelastic neutron scattering reveals details of the shapes of interaction potentials

# Vibrational spectroscopy

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**Complementary to infrared and Raman.**

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**No selection rules:- interaction is with nucleus *not* electrons.**

# Vibrational spectroscopy

**Complementary to infrared and Raman.**

**No selection rules:- interaction is with nucleus *not* electrons.**

**Intensities straightforward to calculate:-**
**Since the neutron scattering law is DIRECTLY calculable, computational techniques are the natural partner to neutron spectroscopy**

**$S(Q,\omega)$ = observed intensity of transition at energy $\omega$, $\sigma$ = inelastic cross-section,**
**$Q$ = momentum transfer,**
**$U_\omega$ = amplitude of vibration for the mode at energy $\omega$**
**$U_T$ = total amplitude of motion.**

# Vibrational spectroscopy

**Complementary to infrared and Raman.**
**No selection rules:- interaction is with nucleus *not* electrons.**

**Intensities straightforward to calculate:-**
**Since the neutron scattering law is DIRECTLY calculable, computational techniques are the natural partner to neutron spectroscopy**

$$S(Q,\omega) = \sigma\, Q^2 U_\omega^2 \exp(-Q^2 U_T^2)$$

**$S(Q,\omega)$ = observed intensity of transition at energy $\omega$, $\sigma$ = inelastic cross-section,**
**$Q$ = momentum transfer,**
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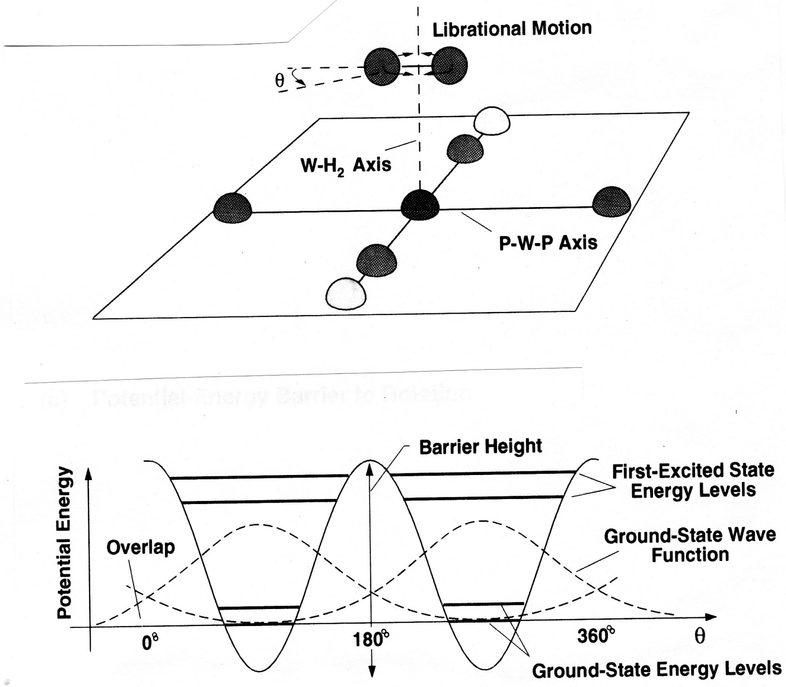
**$U_T$ = total amplitude of motion.**

# Planar Rotation of Molecular Hydrogen

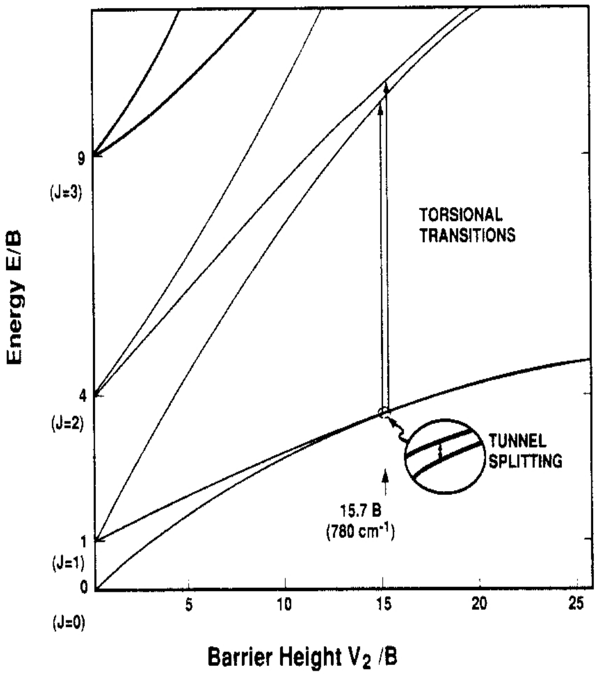
## Model for Dihydrogen Rotation



$$( - B\,\delta^2/\delta^2\varphi \;+\; 1/2\;V_2\cos 2\varphi\;)\;\psi \;=\; E\;\psi$$

$$E_J = BJ^2 \text{ if } V_2 = 0$$

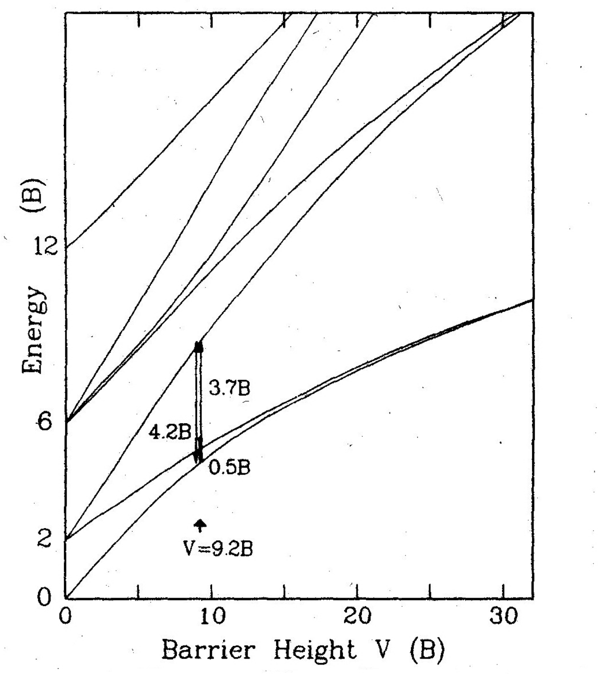
*Molecular Hydrogen Complexes*



Energy level scheme differs appreciably from that for 3-D rotation

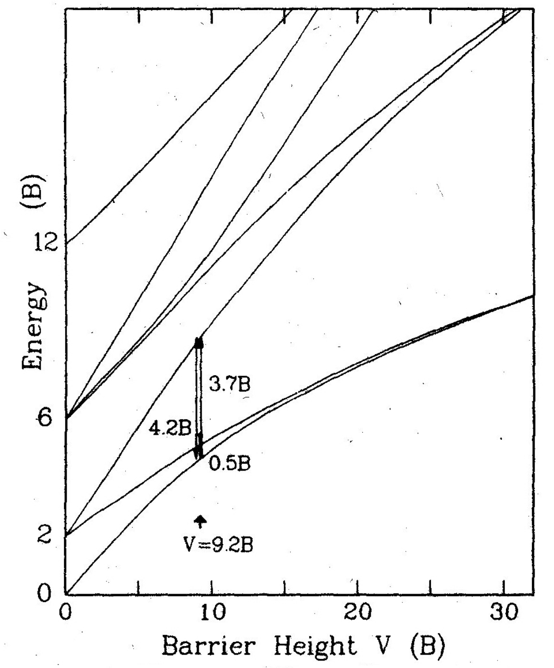
Deduce chemical binding of $H_2$?

# Rotational Tunneling Spectroscopy

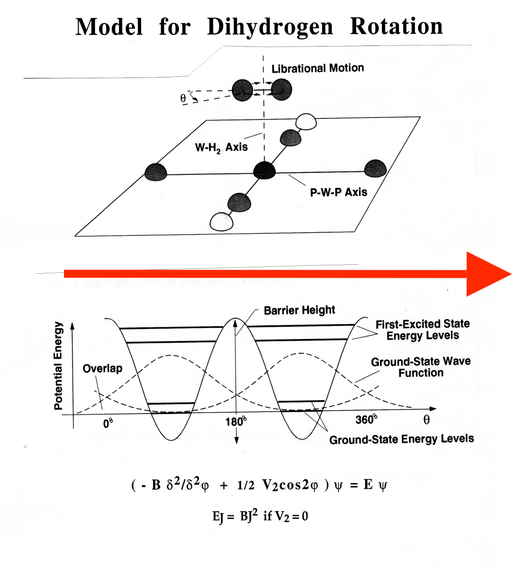


Rotational energy levels for unrestricted 3D rotation of $H_2$

# Rotational Tunneling Spectroscopy



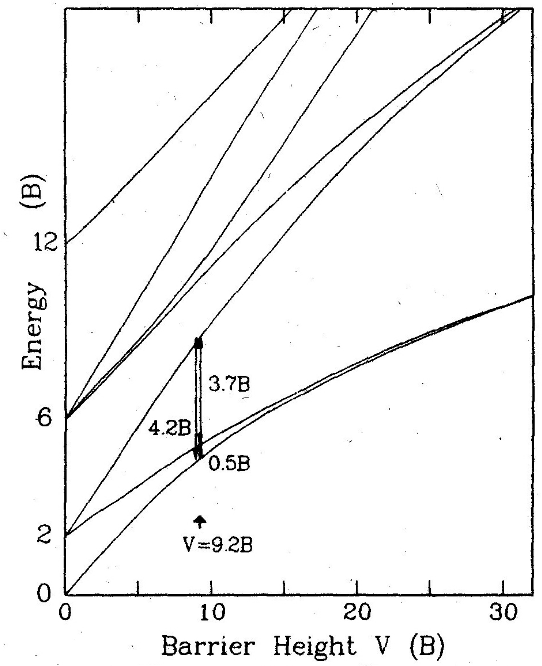
Rotational energy levels for unrestricted 3D rotation of $H_2$


Model for Dihydrogen Rotation

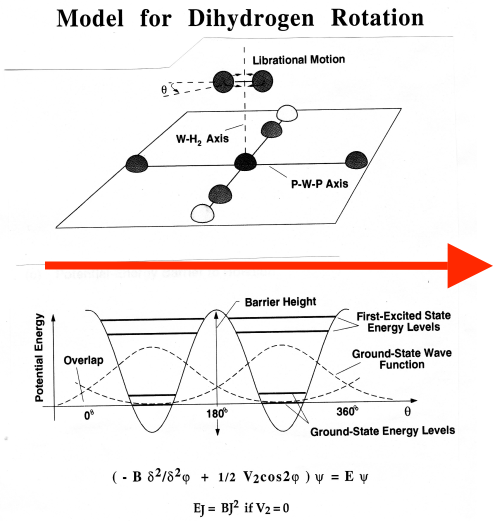
$$( - B\, \delta^2/\delta^2\varphi \; + \; 1/2\; V_2 \cos 2\varphi\; )\; \psi \;=\; E\; \psi$$

$$E_J = BJ^2 \text{ if } V_2 = 0$$

# Rotational Tunneling Spectroscopy



Rotational energy levels for unrestricted 3D rotation of $H_2$



Model for Dihydrogen Rotation

$$(-B\,\delta^2/\delta^2\varphi + 1/2\ V_2\cos 2\varphi)\,\psi = E\,\psi$$

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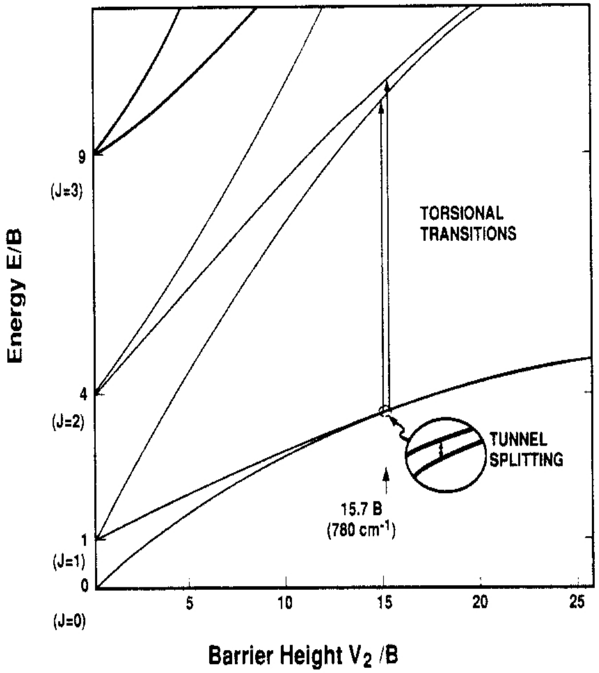
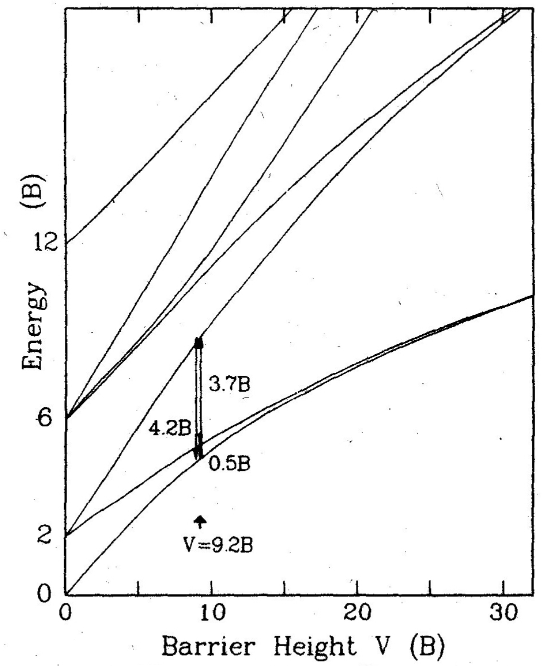
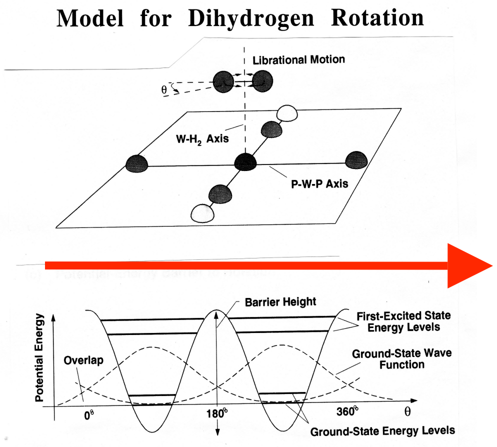


Restricted 2D rotation of $H_2$

# Rotational Tunneling Spectroscopy



Rotational energy levels for unrestricted 3D rotation of $H_2$


Model for Dihydrogen Rotation

$$( - B\, \delta^2/\delta^2\varphi \;+\; 1/2\; V_2 \cos 2\varphi\, )\, \psi = E\, \psi$$

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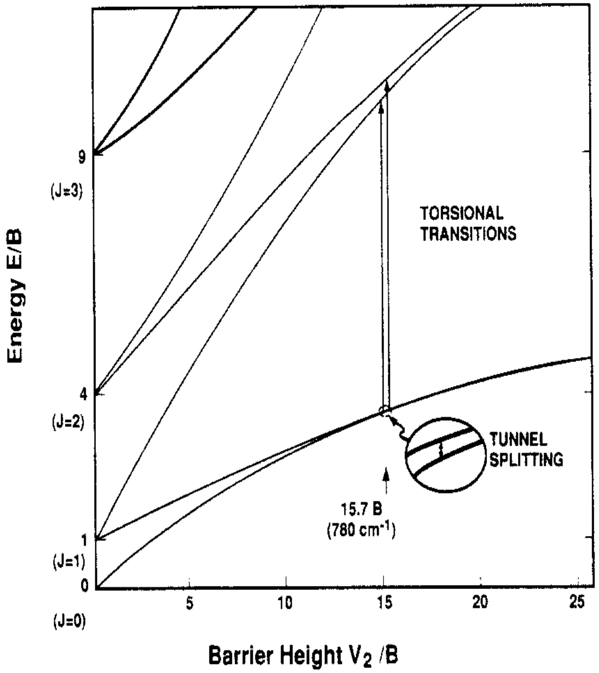
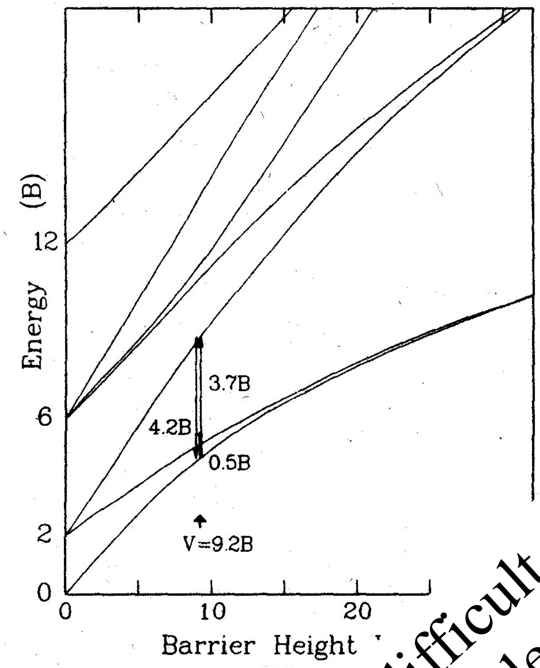


Restricted 2D rotation of $H_2$

Energies typically range between 0.025- 30 meV

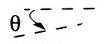
**- How do we measure this?**

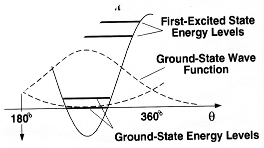
# Rotational Tunneling Spectroscopy



Rotational ener
unrestricted 2 ... 2

Model for Dihydro

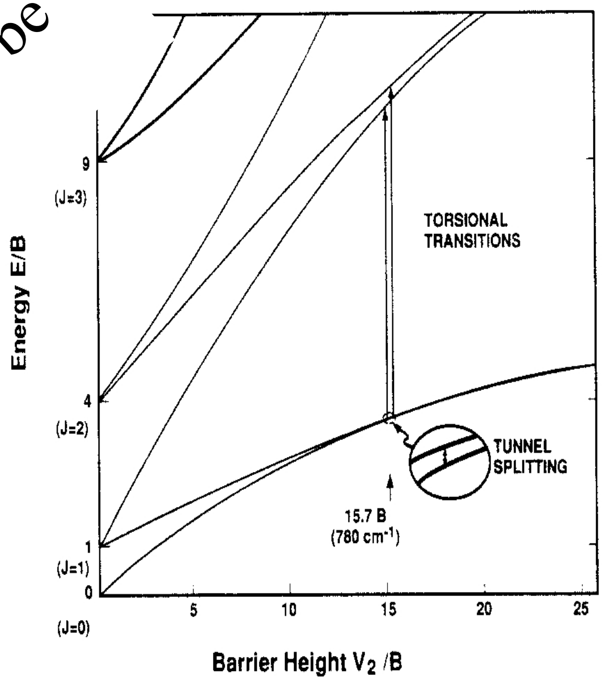




$( - B\, \delta^2/\delta^2\varphi + 1/2\, V_2 \cos 2\varphi )\, \psi = E\, \psi$

$E_J = BJ^2$ if $V_2 = 0$

This is difficult to observe spectroscopically and selection rules in Raman do not allow these to be observed

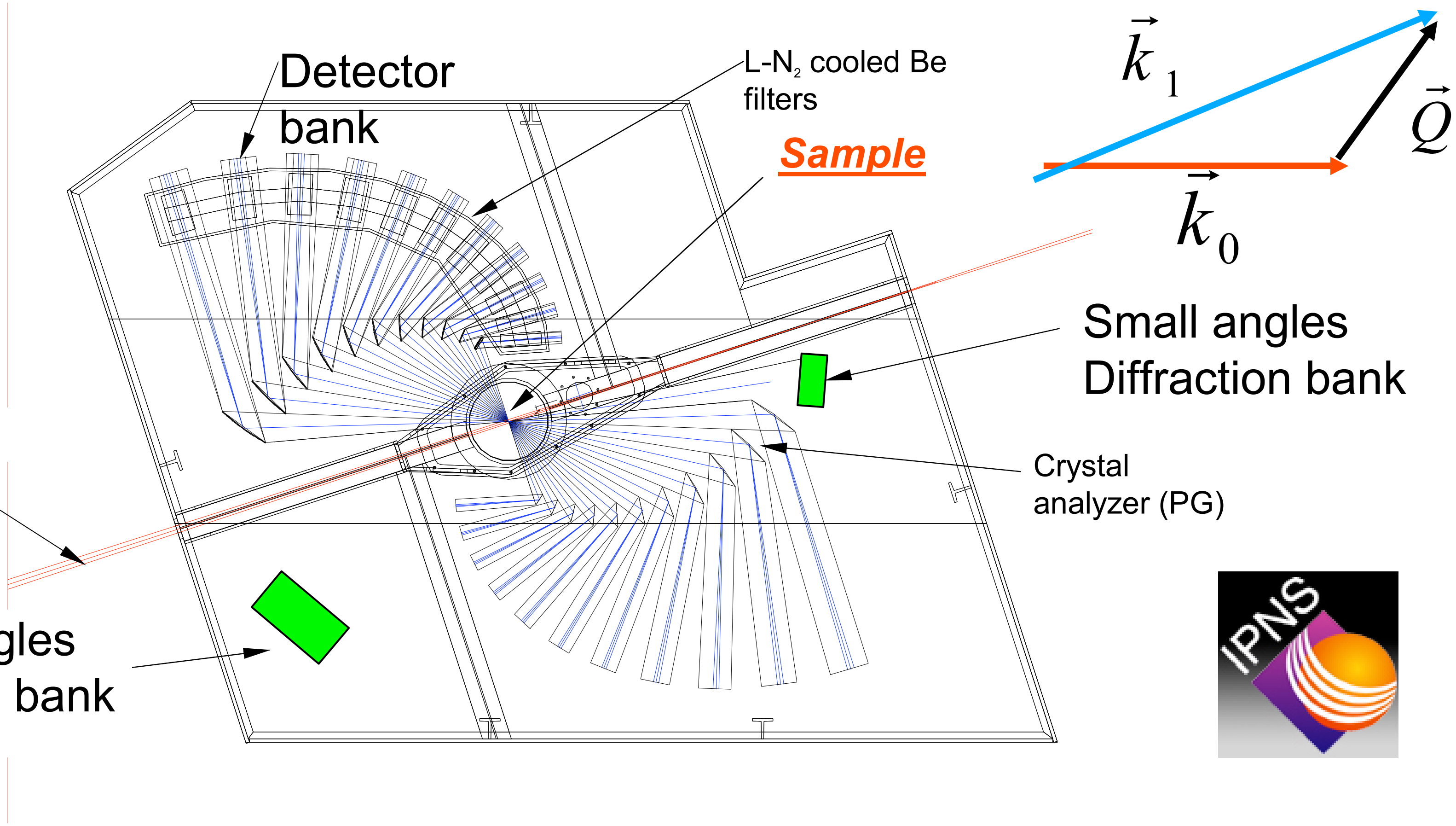


Restricted 2D rotation of $H_2$

Energies typically range between 0.025- 30 meV

**- How do we measure this?**

# QENS



146 detectors

Detector bank

$L\text{-}N_2$ cooled Be filters

***Sample***

$\vec{k}_1$

$\vec{Q}$

$\vec{k}_0$

Small angles Diffraction bank

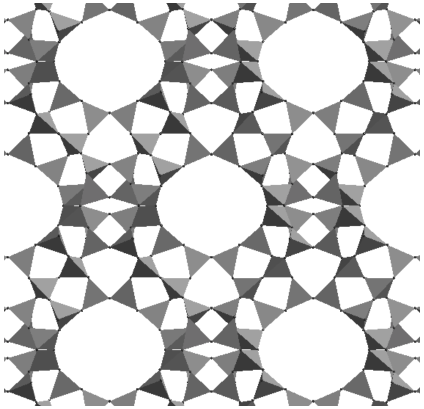
Crystal analyzer (PG)

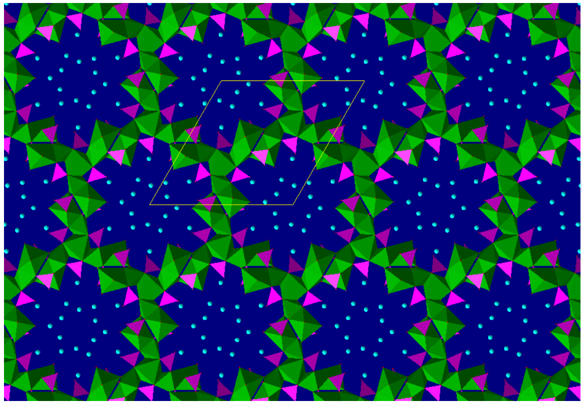
Incident Neutron beam

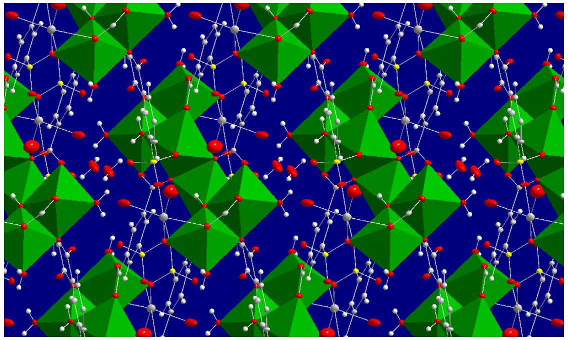
High angles Diffraction bank

# It’s not just surface area:

## hydrogen uptake in porous systems.



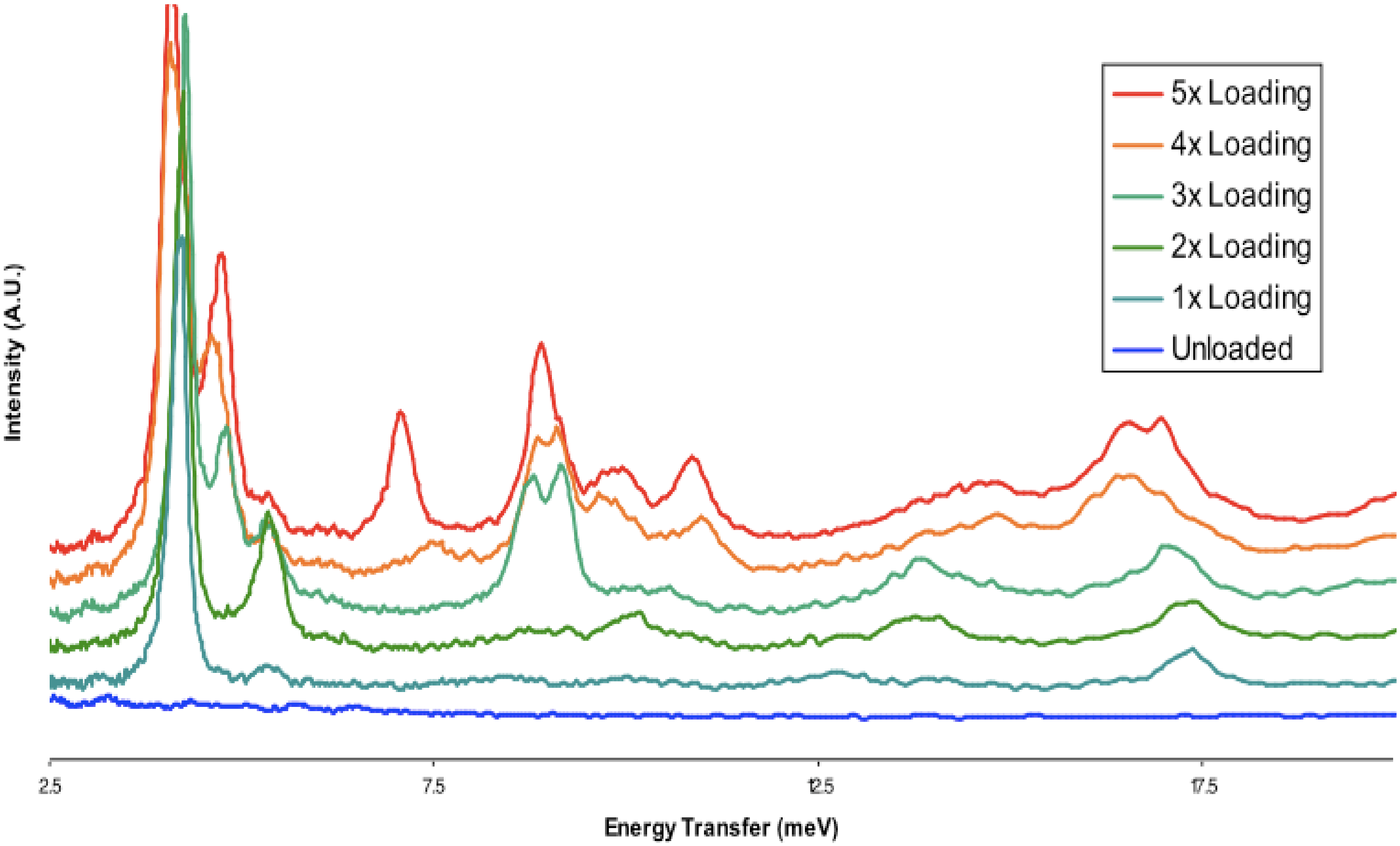




**Paul M. Forster**
Juergen Eckert
Jong-San Chang
Anthony K. Cheetham
John B. Parise.

International Symposium on Materials Issues in Hydrogen Production and Storage, August 25, 2006

# QENS Data



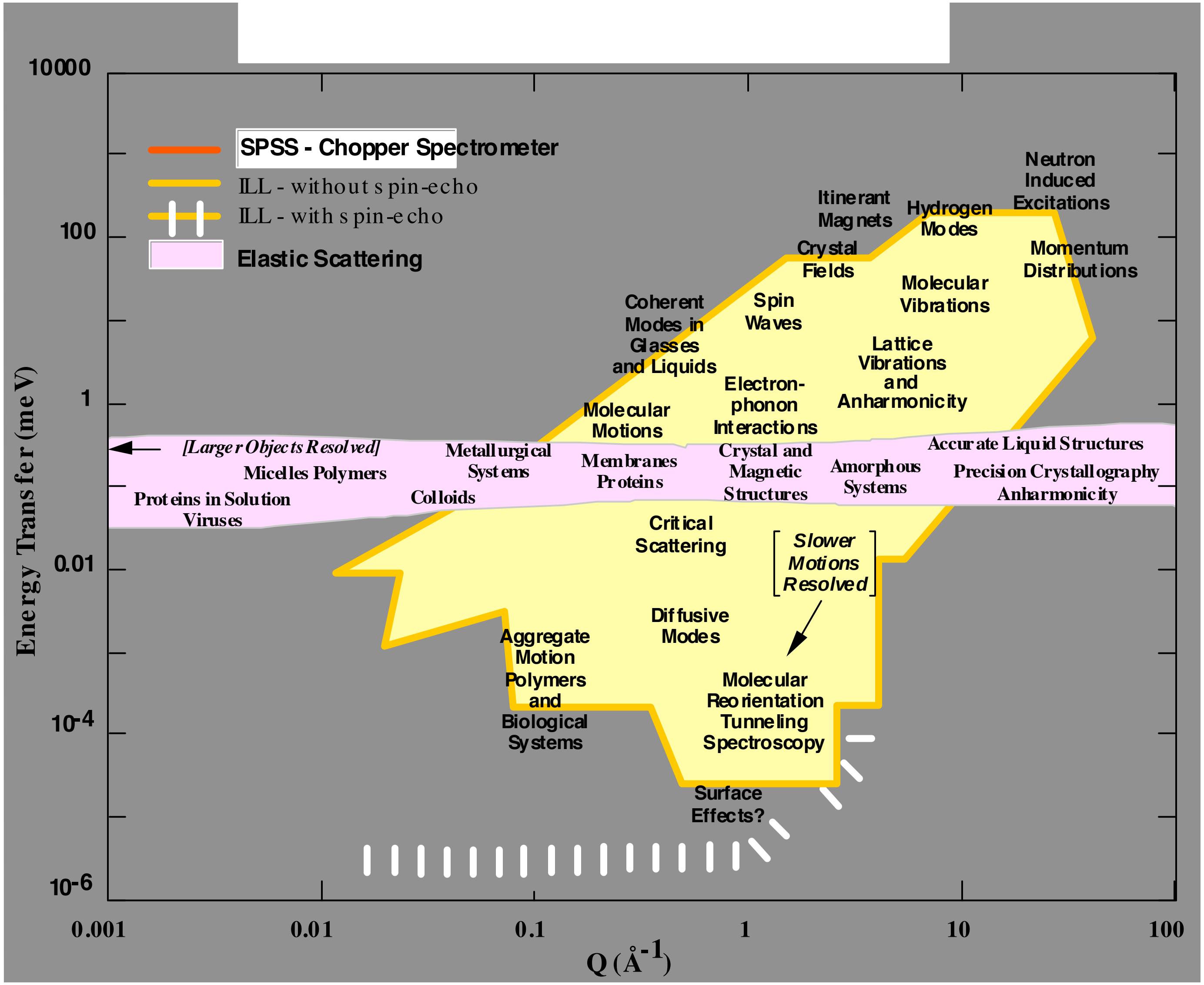
P. M. Forster, J. Eckert, A. K. Cheetham

# Conclusions

- Neutrons have distinct advantages over all length scales of interest to earth and material scientists
  - Imaging and scattering
- Focusing and detector development (and new sources)
  - Increase neutrons on sample
  - Smaller single crystals/powder samples
  - New environmental equipment designs (P, T, $s, e$) measurements
- Prospect of
  - Work on “real” rocks and cores, slurries, in situ pilot plant studies
  - Under variety of conditions

# Phenomena neutrons see: www.mrl.ucsb.edu/~pynn/Lecture_6_Inelastic.pdf

STONY BROOK
STATE UNIVERSITY OF NEW YORK



Energy & Wavevector Transfers accessible to Neutron Scattering

# Future

- Smaller samples
- higher through-put