# Can we determine the grain composition of the Interstellar Medium with Chandra and Astro E2 ?

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with
Bruce Ravel ( NRL )

# Motivation for Dust Studies

- Gets in the way of everything

- Vital to our understanding of the universe
  - dust a primary respository of the ISM
  - chemical evolution of stars, planets, life

`We are stardust ' - Joni Mitchell, Woodstock (Ladies of the Canyon) - 1970

# Multiwavelength studies of dust

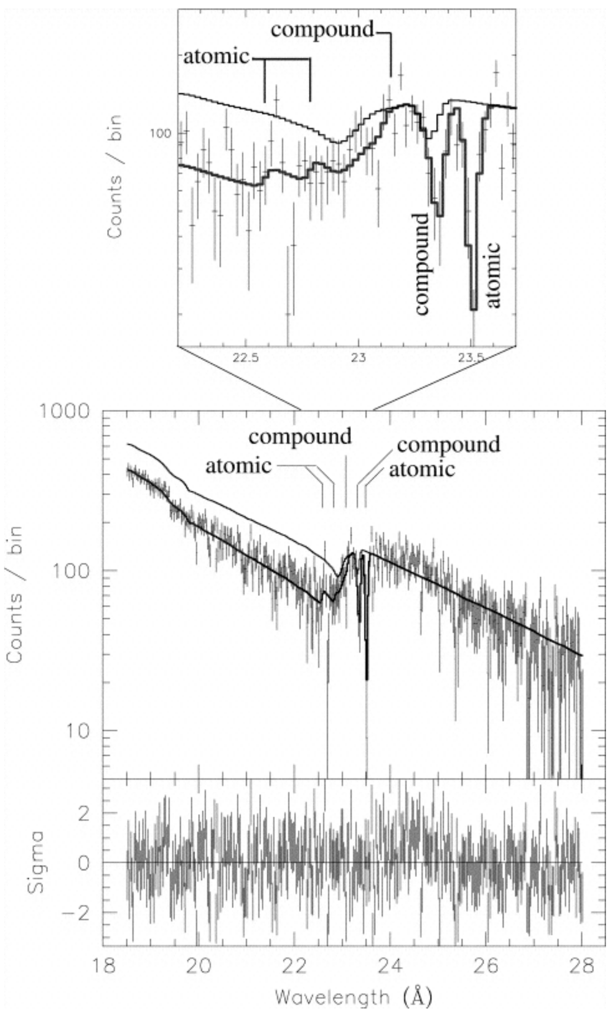
- X-rays : can probe solid state of molecule; sensitive to ALL atoms in both gas and solid phase (as long as grains are ~0.1-1μm)
- IR : can directly probe vibrational modes, but limited to PAHs, graphites and certain silicates (~2.5-25 μm region). Cannot easily speciate the grain composition
- UV : dust inferred from the depletion factor (amount expected : measured)
- Optical : dust inferred from redding/extinction, polarization
- Radio : probe gas phase; 21cm, CO, etc.

# Reviews, etc from some of the experts

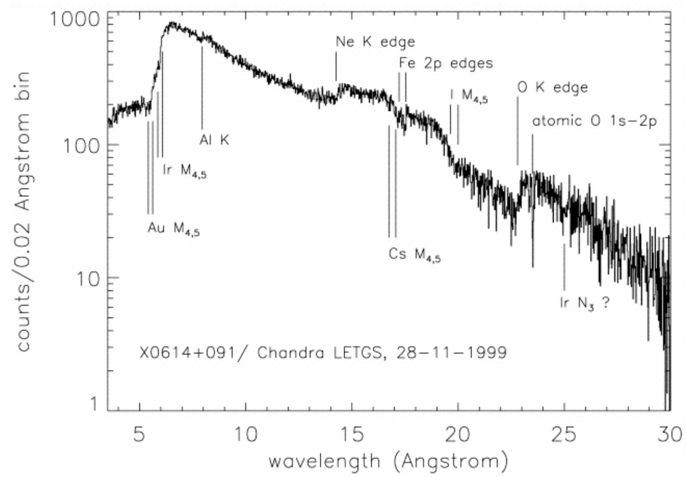
- Dust and Astrophysics :
  - Bruce Draine : Annual Reviews of Astronomy & Astrophysics & references therein
  - Endrik Krügel : `The Physics of Interstellar Dust'
  - Lyman Spitzer : `Physical Processes in the ISM'
  - D C B Whittet : `Dust in the Galactic Environment'
  - Also, ApJ papers by Woo et al. 1995, 97; Forrey et al. 1998
- XAFS Theory & Practice
  - Koningsberger & Prins (1988)
  - Kruegel (2003)
  - B. Ravel & M. Newville
  - Rehr & Albers (2000)
  - J. Stöhr (1996)

# X-ray ISM Studies with X-ray binaries with the Chandra HETGS & LETGS

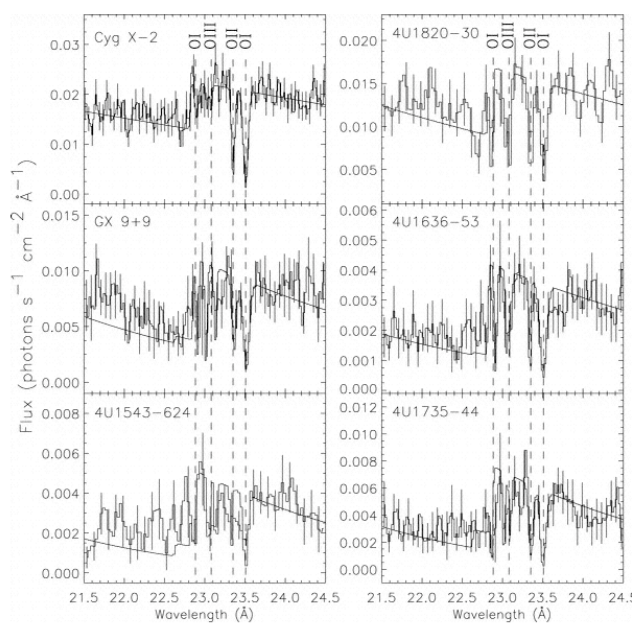
CYG X2 LETGS: Takei et al. 2002




X0614+091 LETGS : Paerels et al. 2001




Oxygen K edges in XRBs : Juett et al. 2004




detect K-shell O, Ne and L shell Fe

1st attempt to measure ISM absorption edges : (detected OI & Ne edges & hint of 1s-2p oxygen resonance in the Crab)

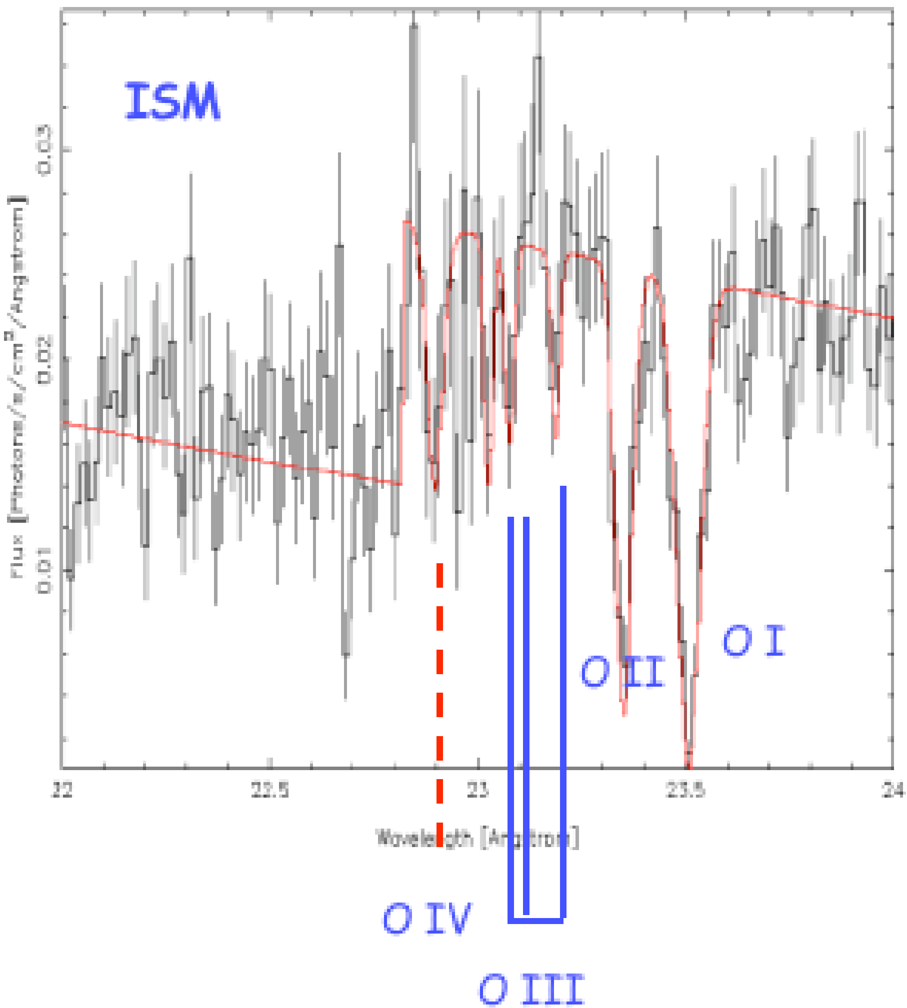
Schattenburg & Canizares 1986

Einstein Focal Plane Crystal Spectrometer

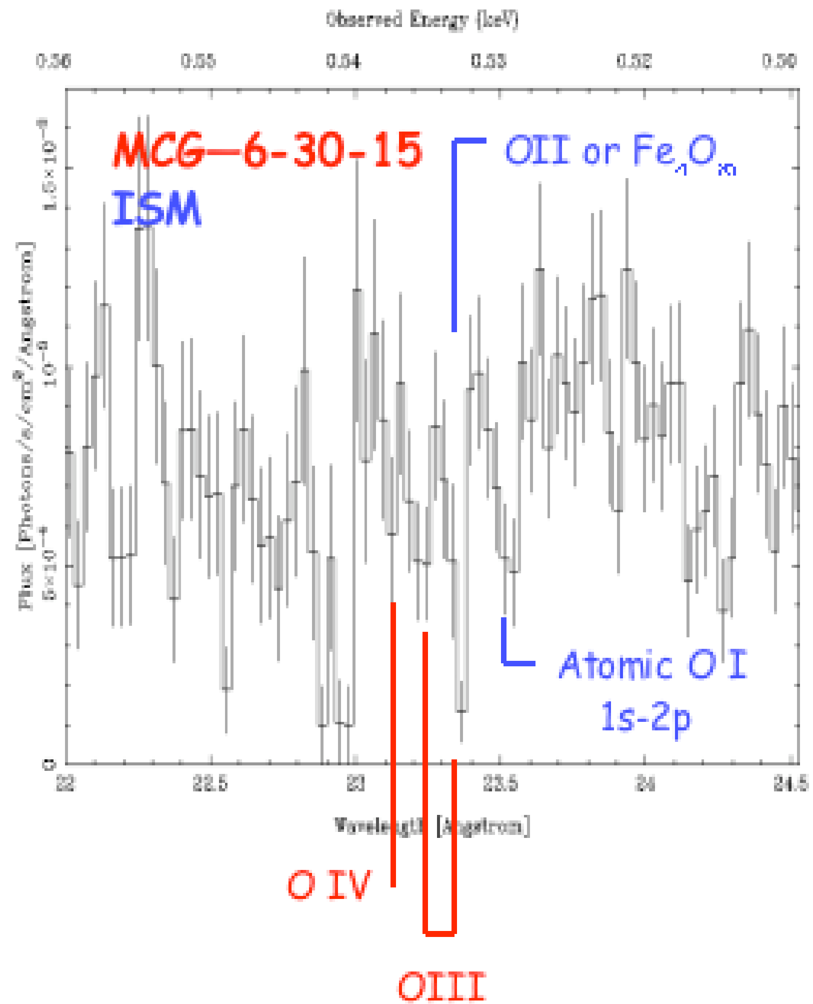
See also Schulz et al. 2002
de Vries 2003

# ISM Studies with Chandra

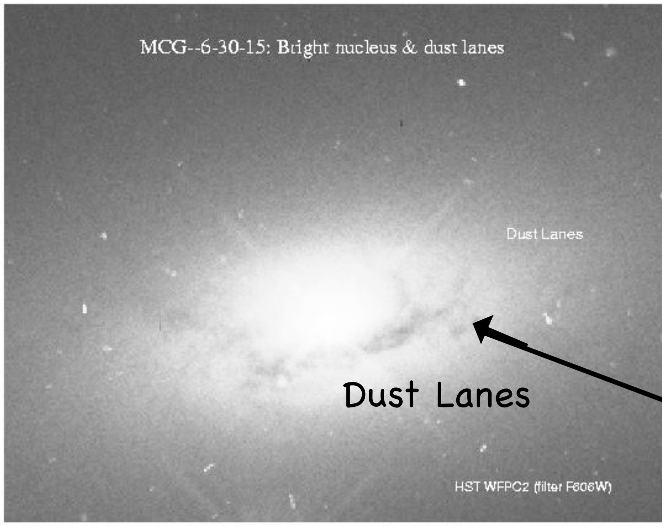
XRB: Cyg X2: Juett et al. 2004

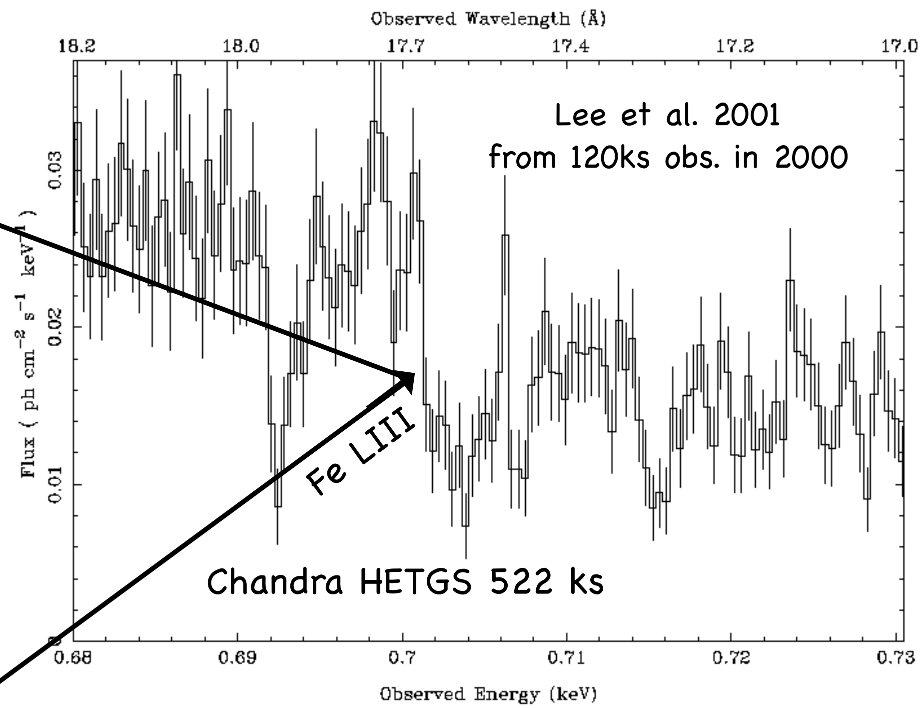


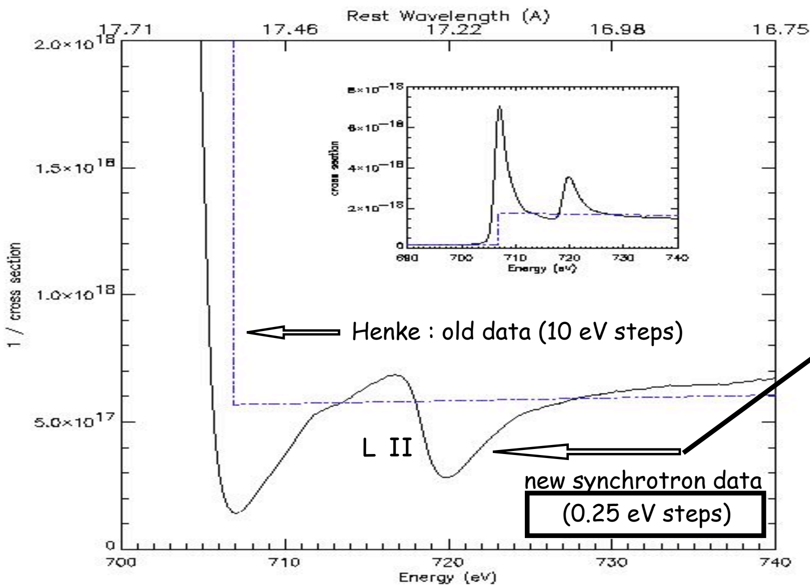

AGN: MCG-6-30-15 : Lee et al., in prep.



# Dust embedded in the ionized absorber of Seyfert galaxy MCG-6-30-15



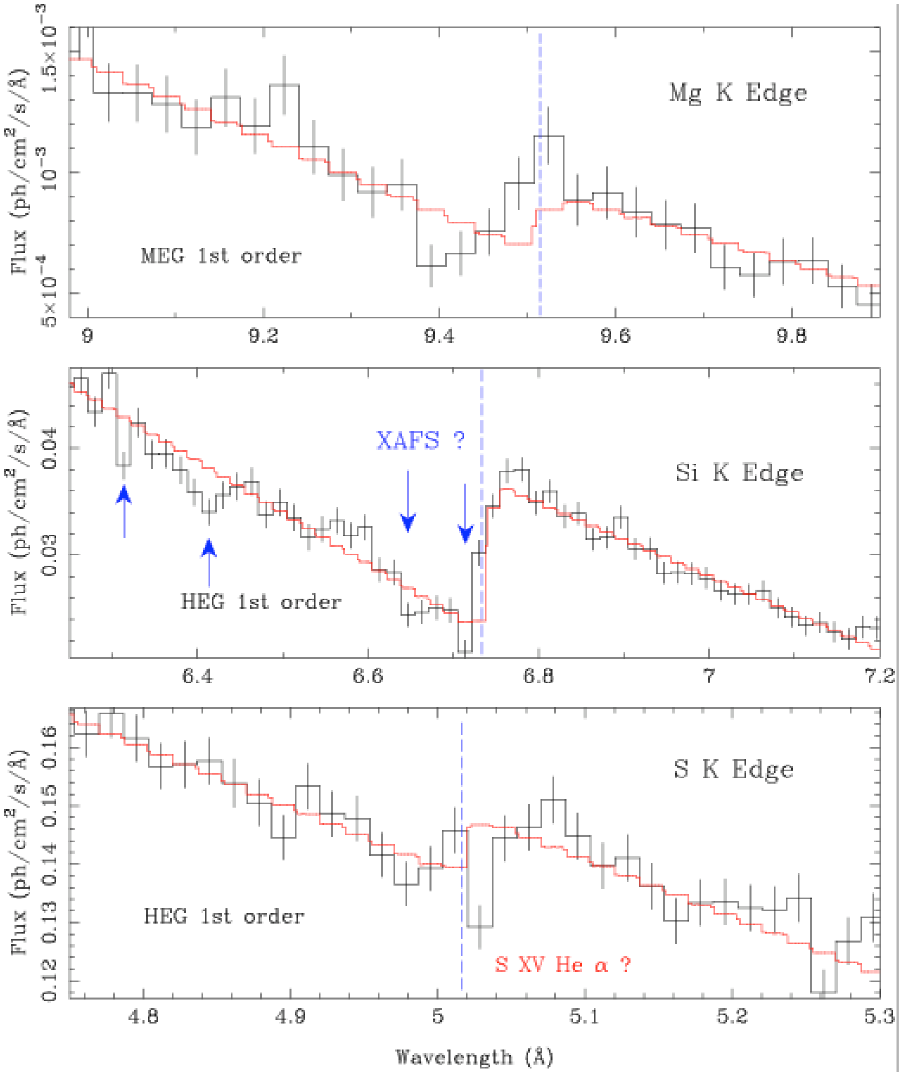

$\tau_{\mathrm{FeI\ LIII}} \rightarrow N_H \sim 4 \times 10^{21}\ \mathrm{cm}^{-2}$

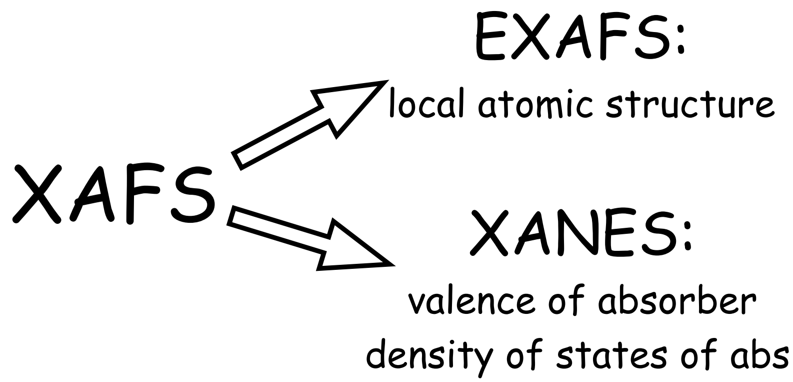
$E(B-V) = 0.69\text{–}1.09 \rightarrow N_H \sim 4 \times 10^{21}\ \mathrm{cm}^{-2}$

- Kortright & Kim 2000 Phys Rev B, 62, 1226 (New laboratory measurements)
- also Ming Feng Gu : new calculation

# Detections of X-ray Absorption Fine Structure

GRS 1915+105 : Lee et al. 2002a




- interstellar grain composition
- solid state astrophysics ?!

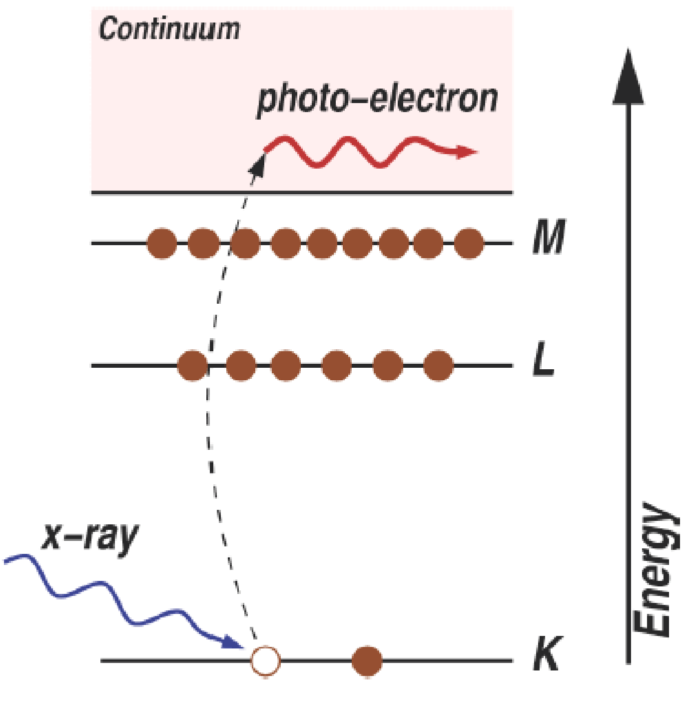
# The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

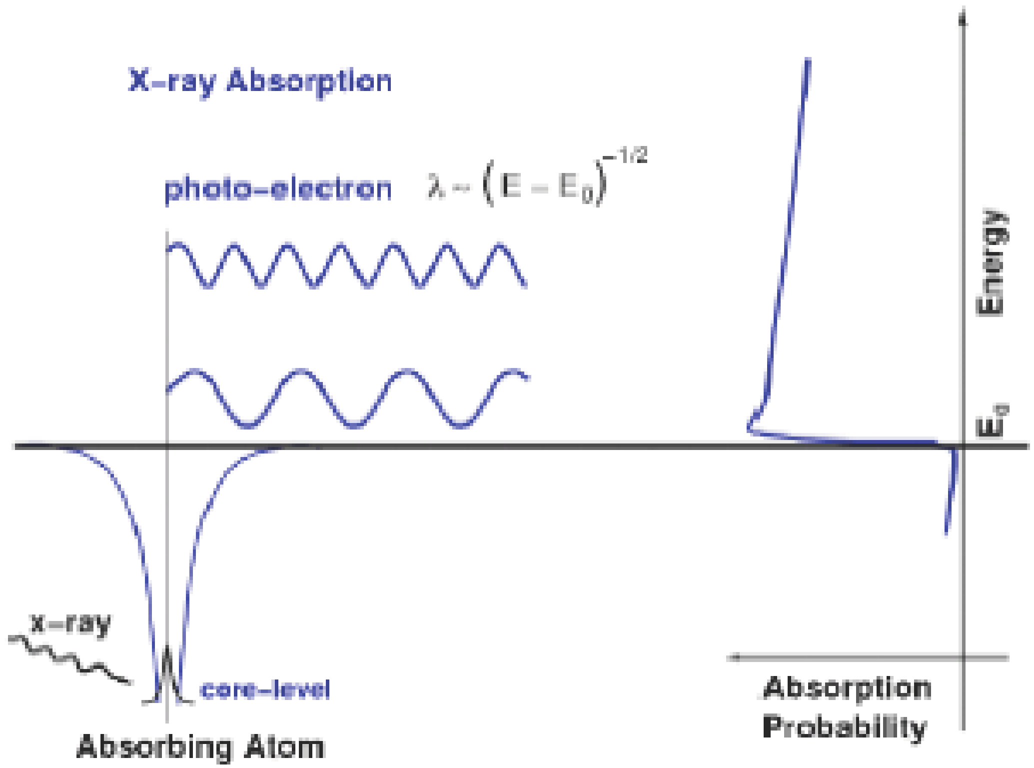
- The photoelectric effect : X-ray photon absorbed by an electron in a tightly bound quantum core level (e.g. 1s or 2p)

# Bound-free case for isolated atoms

## X-ray absorption through the photoelectric process

Isolated Atom: Bound free process --> edge step



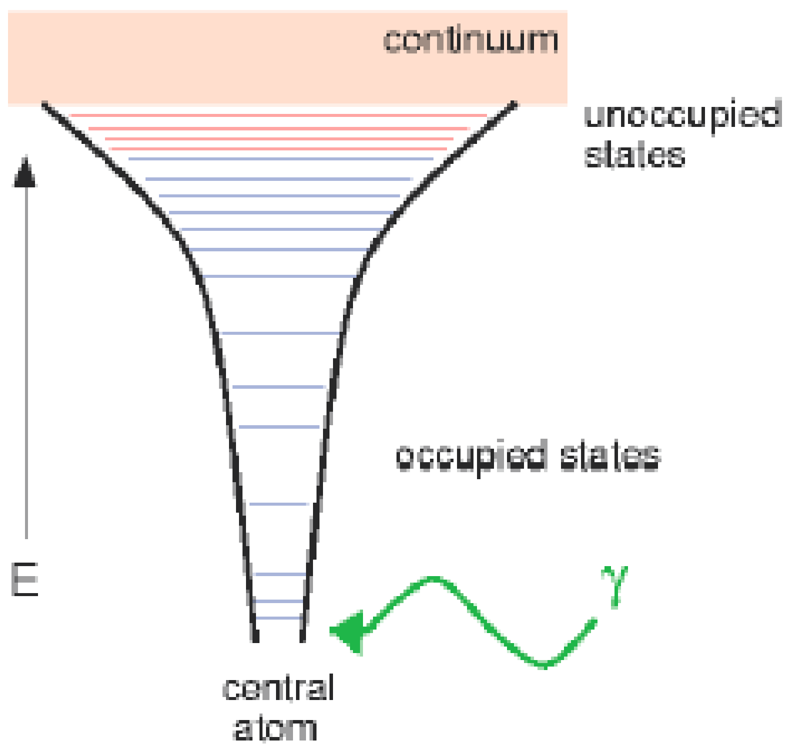



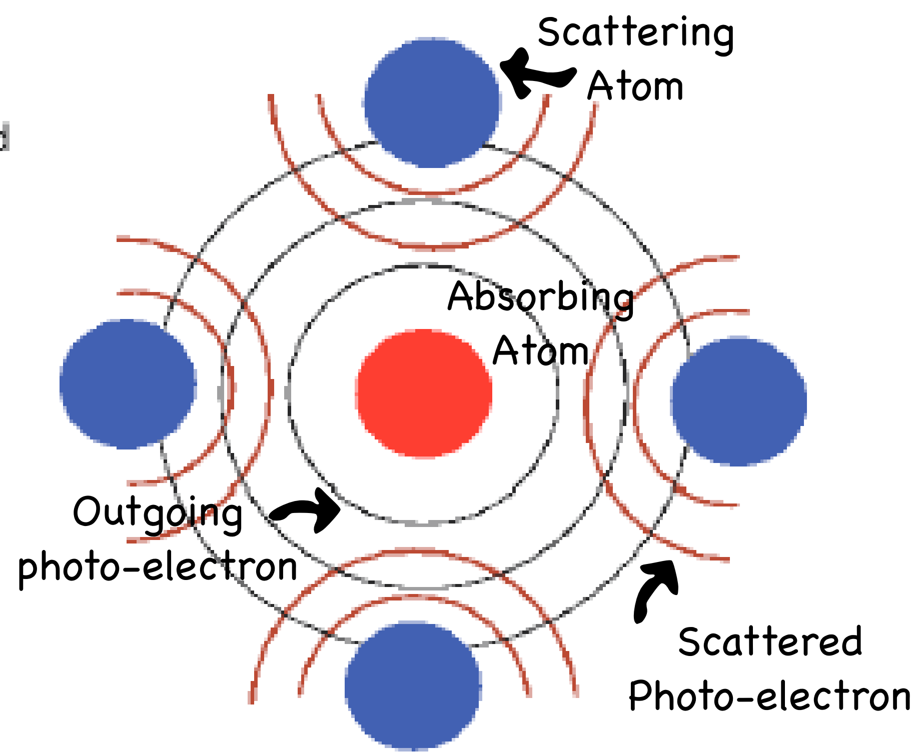

Figures from "XAFS" : © 2002 Matt Newville

# The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

- The photoelectric effect : X-ray photon absorbed by an electron in a tightly bound quantum core level (e.g. 1s or 2p)
- Isolated Atom: Bound free process --> edge step
- Isolated Atom : Bound bound process --> inner shell resonance absorption lines (e.g. MCG-6-30-15: Oxygen V, VI KLL : Lee et al. 2001; IRAS 13349 : 2p-3d M-shell Fe : Sako et al. 2000, NGC 3783 -- Kaspi et al. 2002, Netzer et al. 2003 & references therein)
- Molecule : bound-bound process --> XAFS

# Heuristic Picture of EXAFS



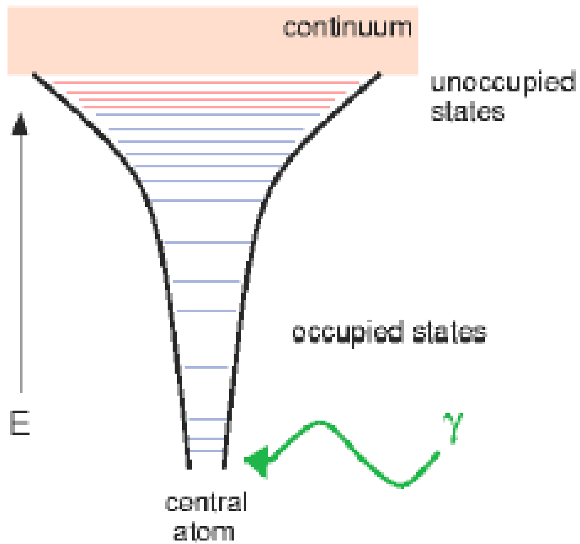



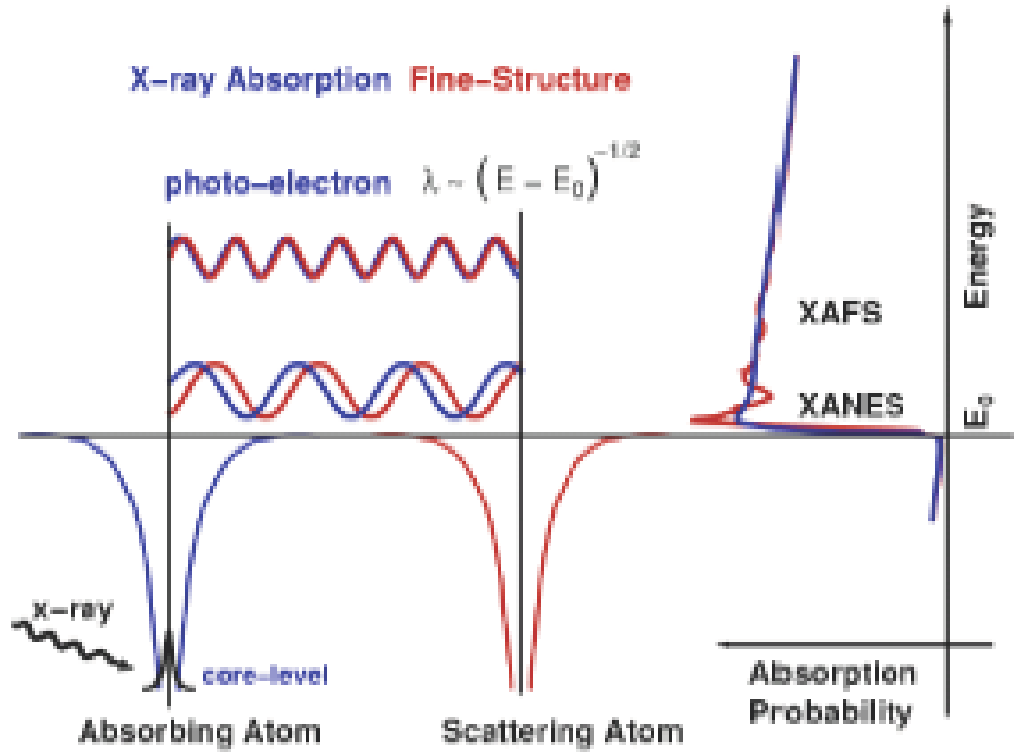

Introduction to EXAFS Analysis Using Theoretical Standard, ©2000-2001 Bruce Ravel

(1) Deep core electron is excited into a state above Fermi energy

(2) Single Scattering Approximation :
The photoelectron propagates as a spherical wave & interacts with neighboring atoms -> backscattered wave

# XAFS Theory
# Bound-bound case for molecules




Figures from "XAFS" : © 2002 Matt Newville

The amplitude of the back-scattered photo-electron at the absorbing atom will vary with energy --> oscillations in μ(E) --> XAFS

# The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

## Fermi's Golden Rule :

initial state : an X-ray, a core electron, no photo-election

↓

$$\mu(E) = \mu_0(E)[1 + \chi(E)] \propto |<i|H|f>|^2$$

↑

final state : no X-ray, a core hole, a photo-election

## Fine-Structure Term :

↓ depends ONLY on absorbing atom

↓ change in photo-electron final state due to back-scattering from neigboring atom

$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E)} \propto <i|H|\Delta f>$$

H: interaction term - represents changing between 2 energy, momentum states

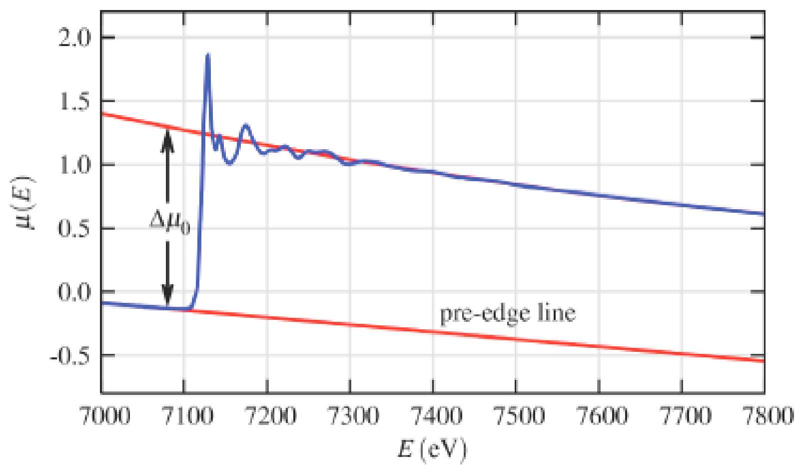
## The EXAFS equation

photo-electron scattering properties of neighboring atoms

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{k{R_j}^2} \sin[2kR_j + \delta_j(k)]$$

Single Scattering Approximation

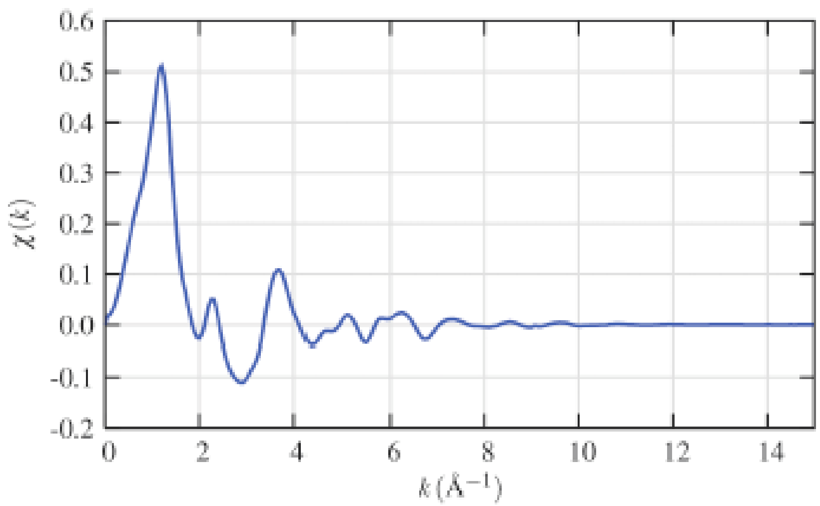
# The practice behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

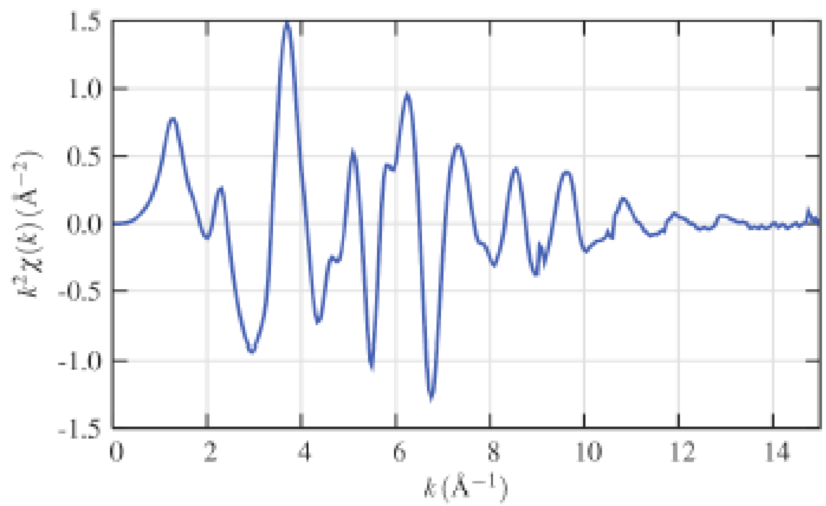



Isolate fine structure term :

$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E)} \propto < i \,|\, H \,|\, \Delta f >$$

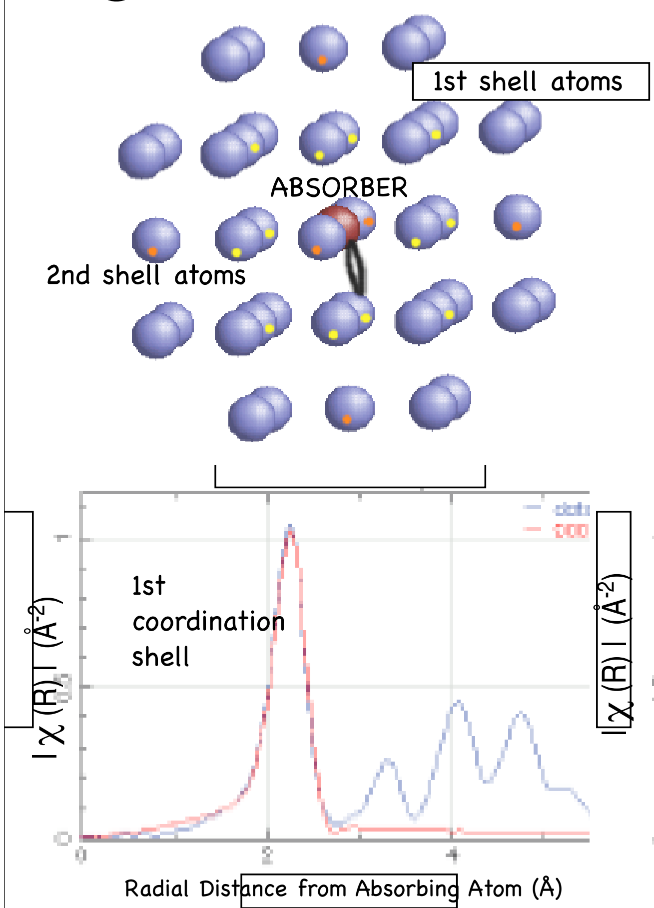
$$\chi(E) \longrightarrow \chi(k) \qquad \mathbf{k} = \sqrt{\frac{2m(E - E_0)}{\hbar^2}}$$



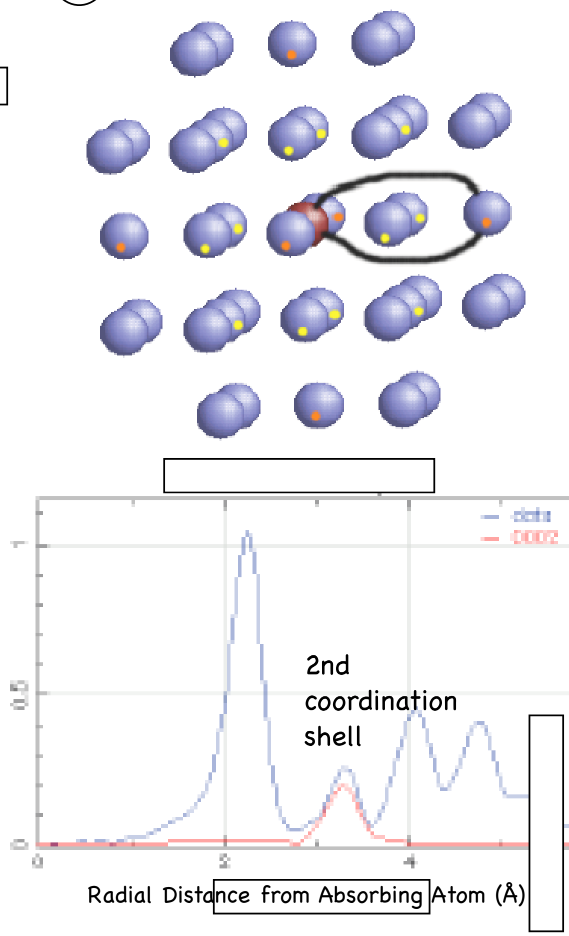



# Scattering Paths

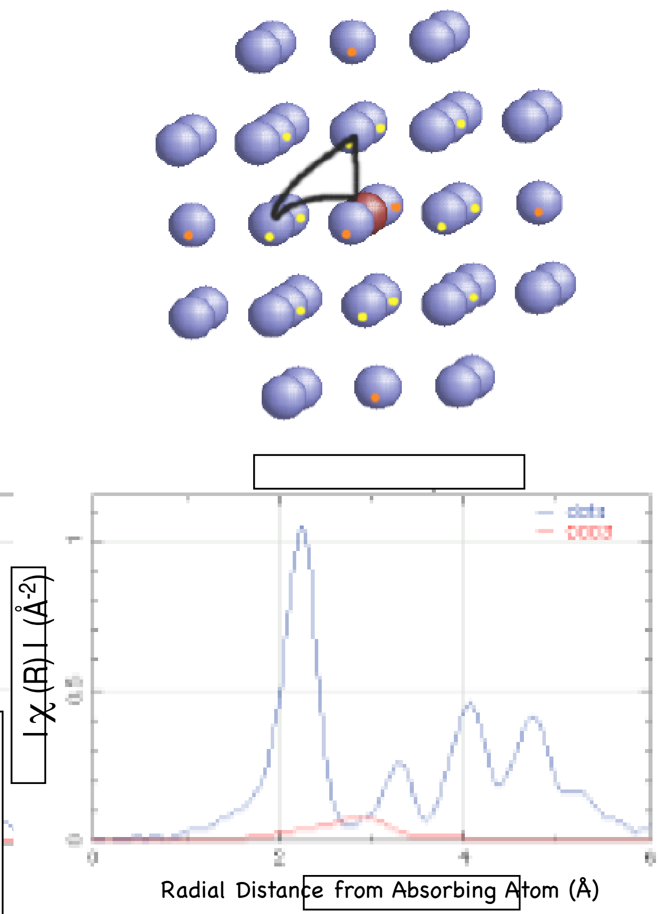
1 Single Scattering Path




2 Single Scattering Path




3 Double Scattering Path ...

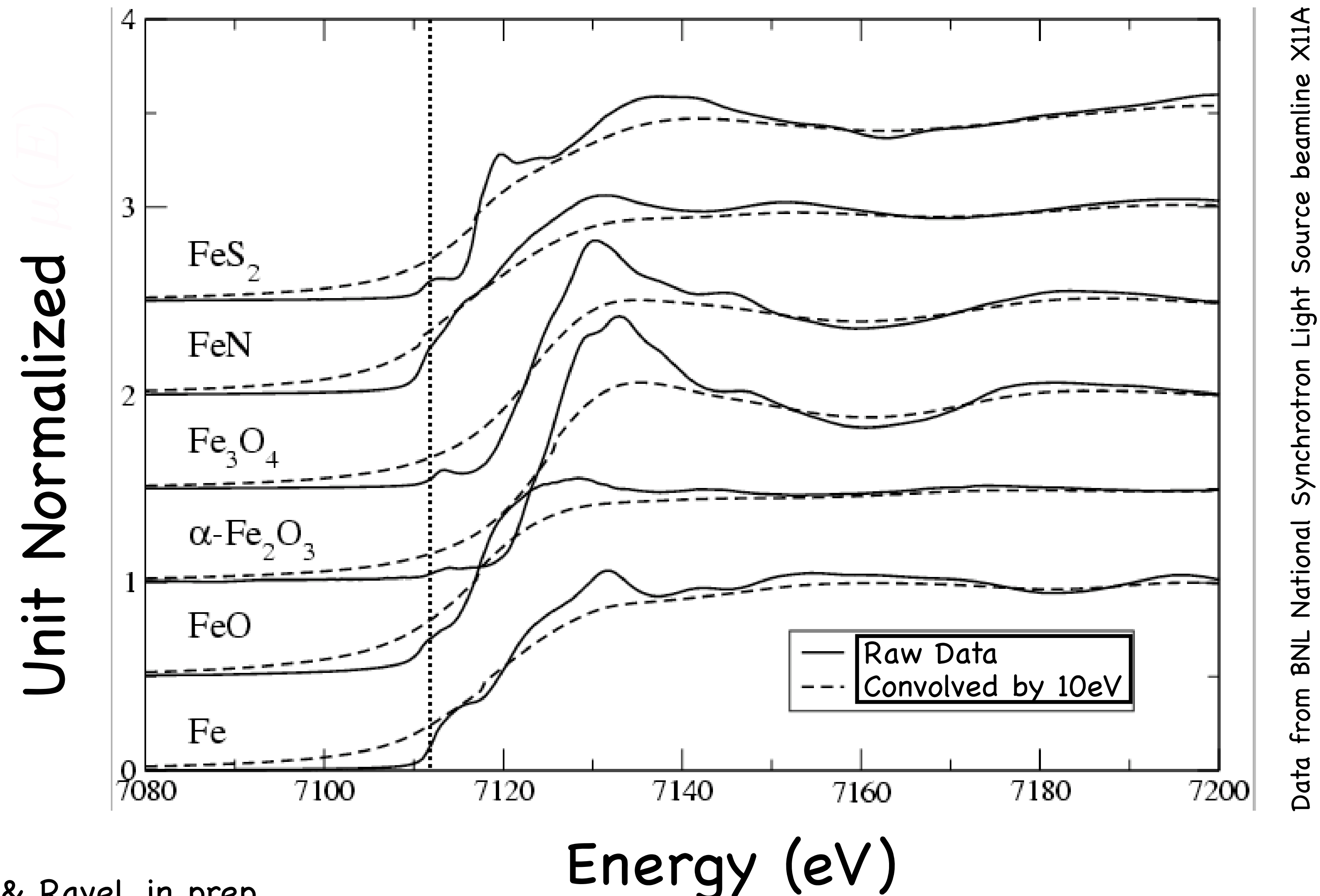



$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} \, e^{-2k^2\sigma_j^2}}{kR_j{}^2} \sin[2kR_j + \delta_j(k)]$$

# ISM Grain Candidates

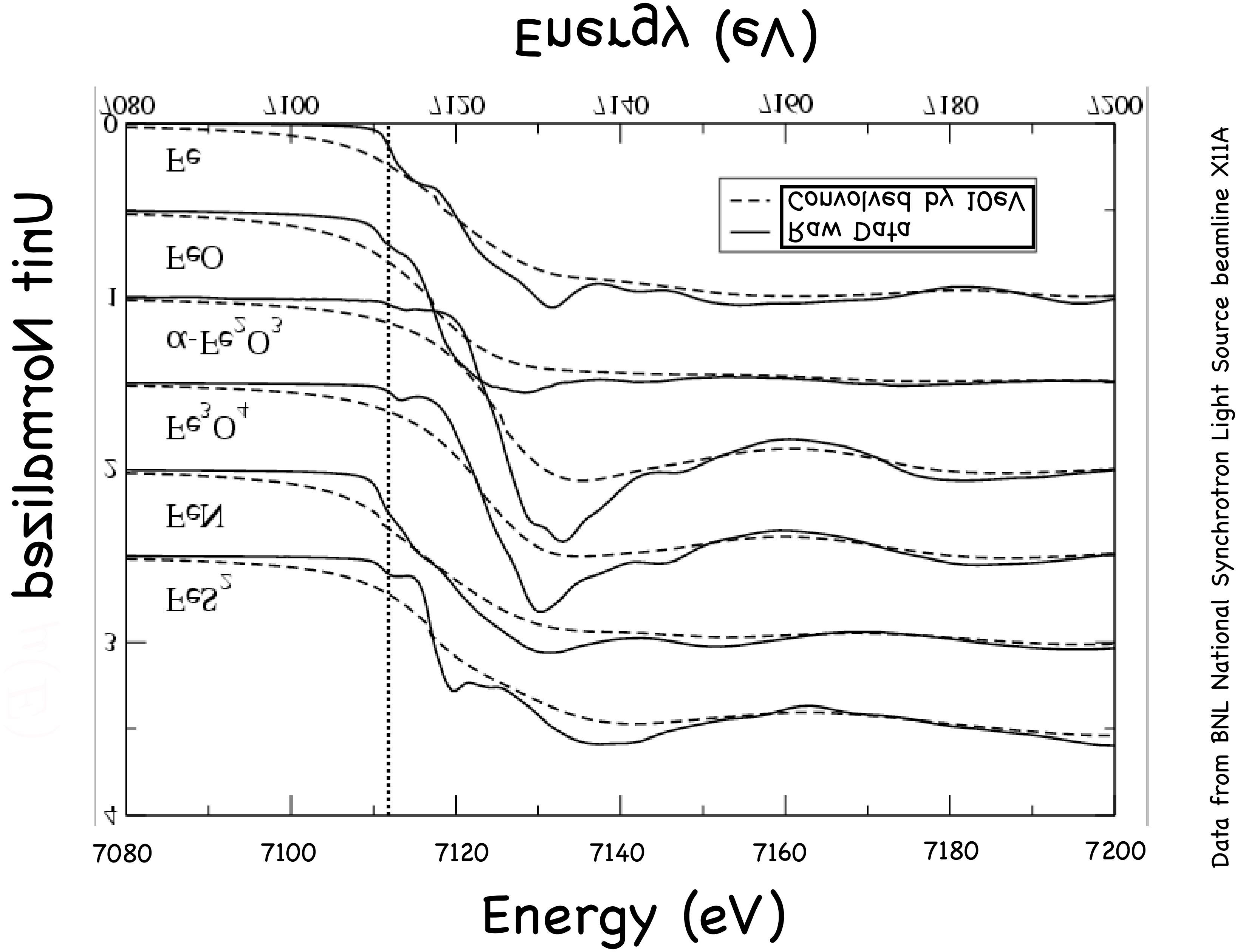
- UV, IR, & meteorite studies indicate compositions :
  - ice : $H_2O$
  - graphite : C
  - polyaromatic hydrocarbons : PAHs
  - silicates : $SiO_2$, $FeSiO_3$, $FeSiO_4$, $MgSiO_3$, $Mg_2SiO_4$
  - iron species : Fe, FeO, $Fe_2O_3$, $Fe_3O_4$

# K-edge Absorption Cross Sections for IRON compounds




Lee & Ravel, in prep.

# For us Astronomers ...

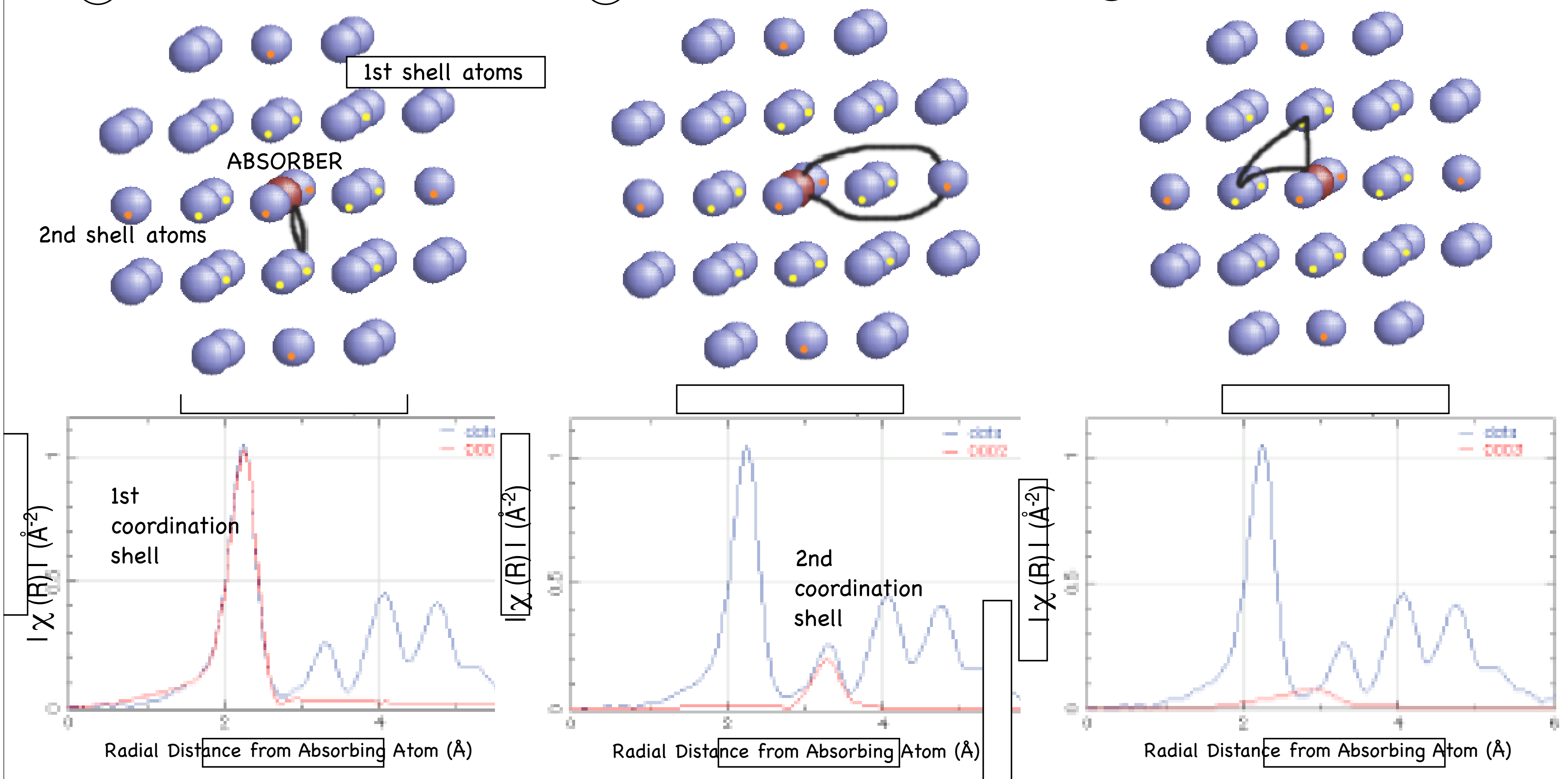


# Scattering Paths

1 Single Scattering Path

2 Single Scattering Path

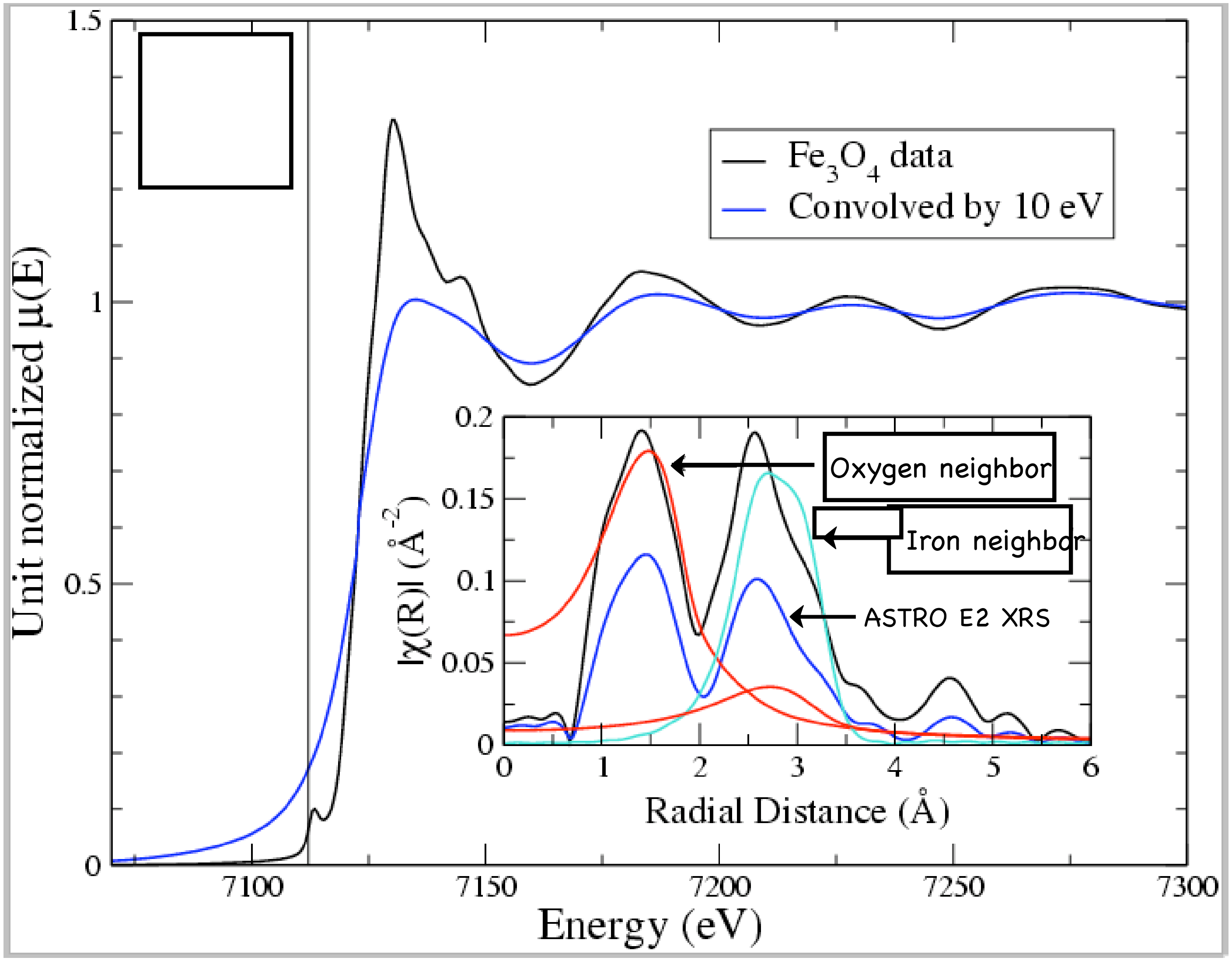
3 Double Scattering Path ...




$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)}\, e^{-2k^2\sigma_j^2}}{kR_j{}^2} \sin[2kR_j + \delta_j(k)]$$

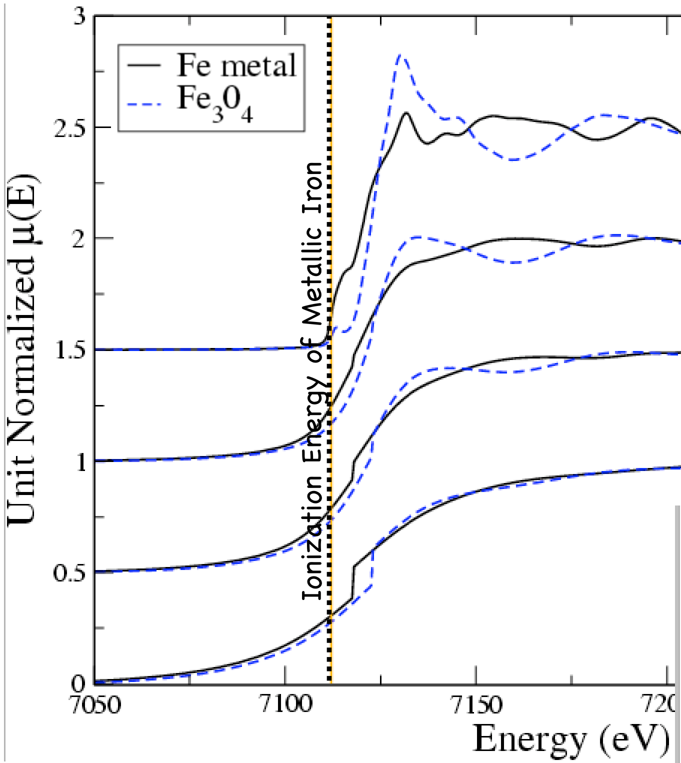
# Identifying Compounds using
# XAFS theory and synchrotron analysis techniques

Data from BNL National Synchrotron Light Source beamlin

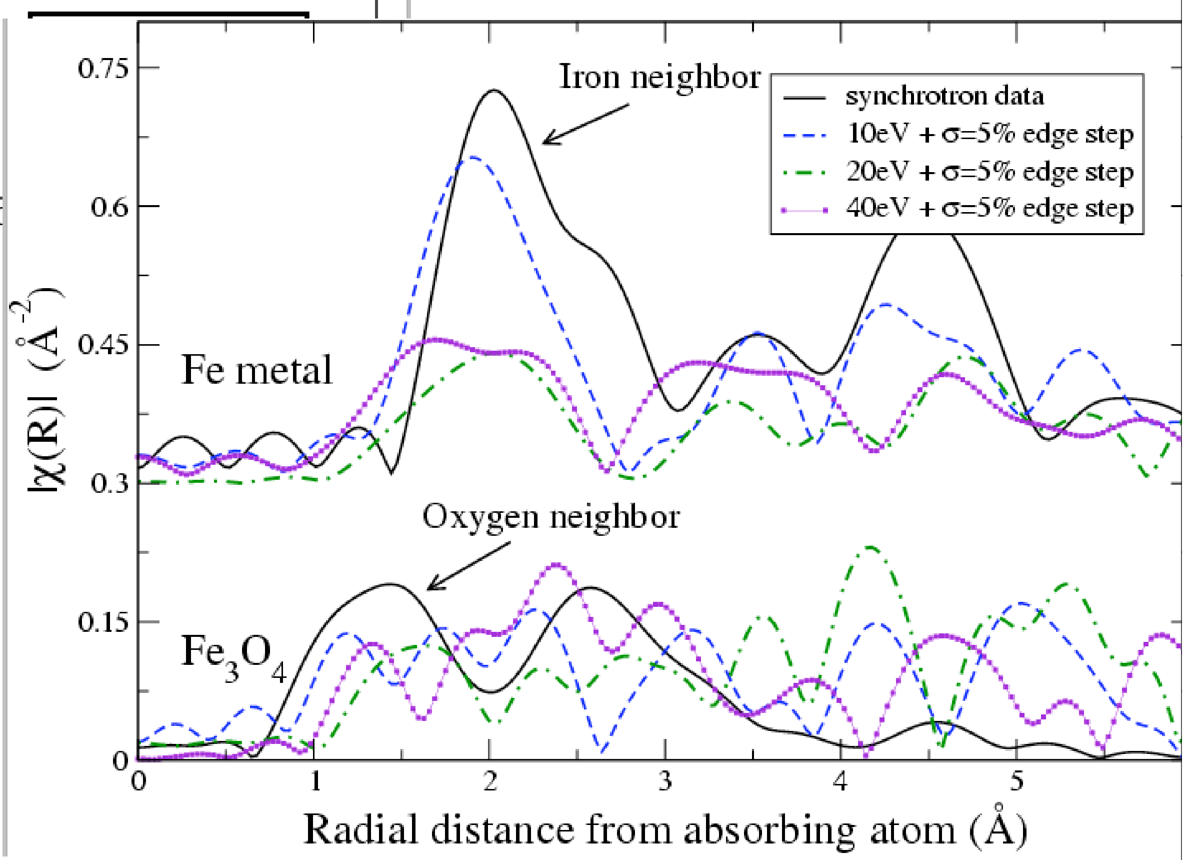



Lee & Ravel, in prep.

Lee & Ravel, in prep.




# The limiting effects of spectral resolution



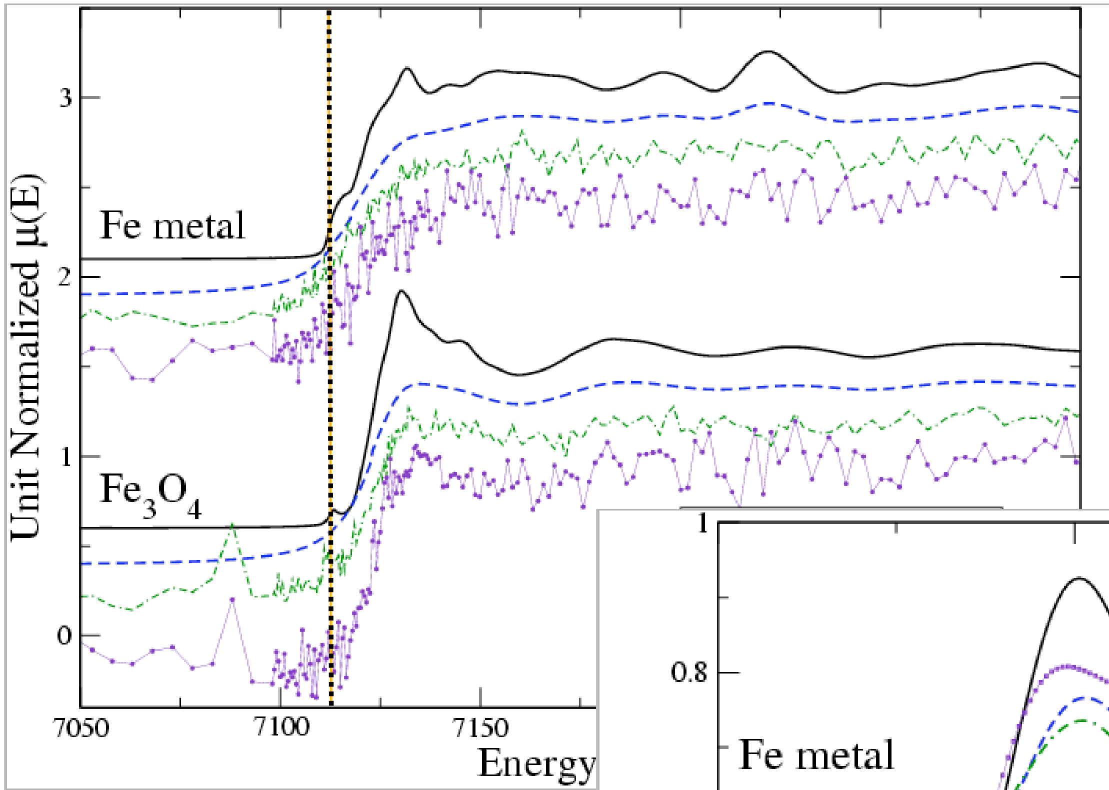

At moderate noise level

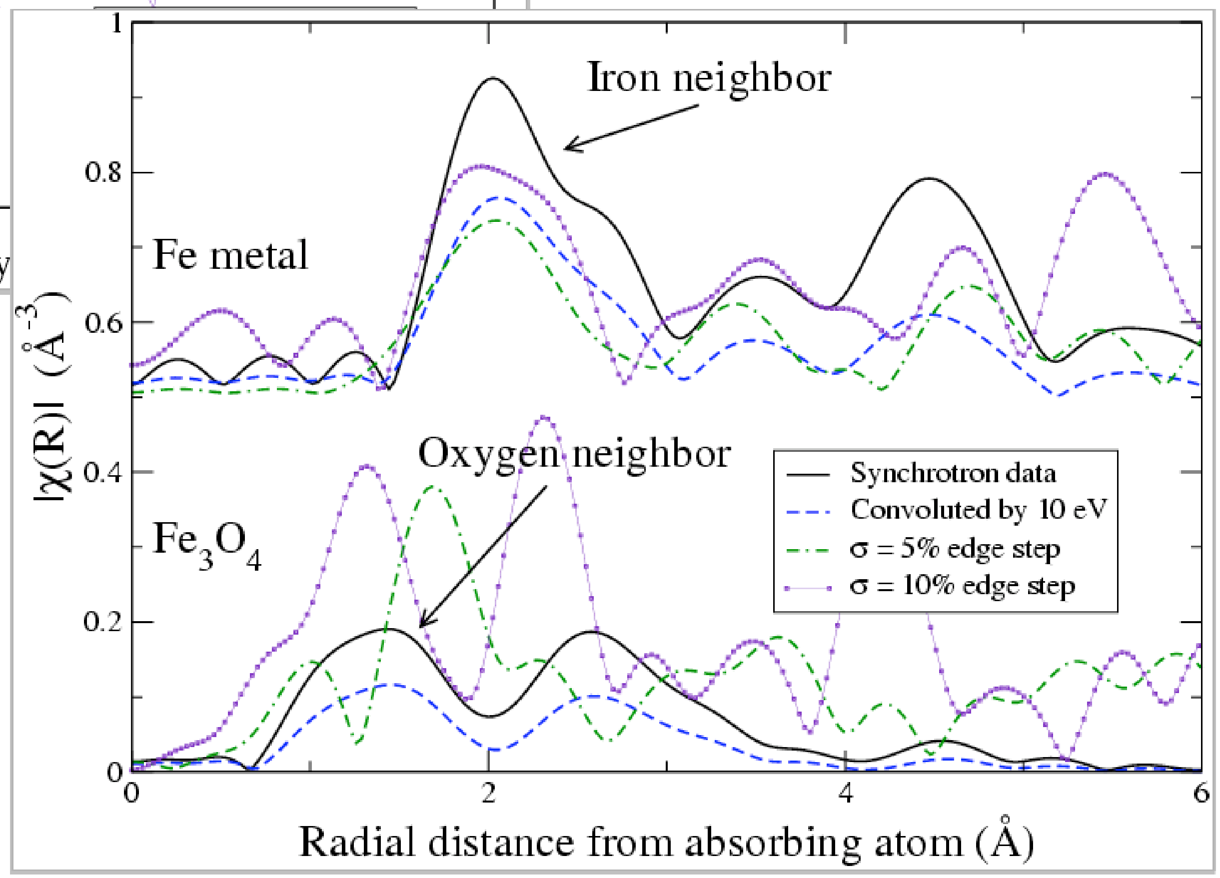
Fe Metal :
R = 20 eV maybe still OK

Magnetite :
R = 10 eV a minimum

Data from BNL NSLS X11A beamline

# The limiting effects of noise




Lee & Ravel, in prep.

<u>At R~10 eV</u>

Fe Metal :
can tolerate relatively high noise

Magnetite :
cannot even tolerate 5% noise

Data from BNL NSLS X11A beamline

# Can we determine the grain composition of the Interstellar Medium with Chandra and Astro E2 ?

- YES but NOISE a serious impediment
  - Difficult in the soft X-rays; other abs. lines
  - Easier with Astro E2 XRS, *if* iron-based dust
  - ** definately will be able to separate gas from dust **
- Space-based measurements should be complemented with empirical XAFS data taken at synchrotron beamlines to determine exact chemical state of the astrophysical dust
- Recent measurements of soft X-ray XAFS at ALS (Sept 04)
- FUTURE MISSIONS : area + spectral resolution