New Opportunities in Fundamental Atomic Physics, Solid State Theory, Experiment and Synchrotron Science, including Discovery of new satellites using extended range HERFD

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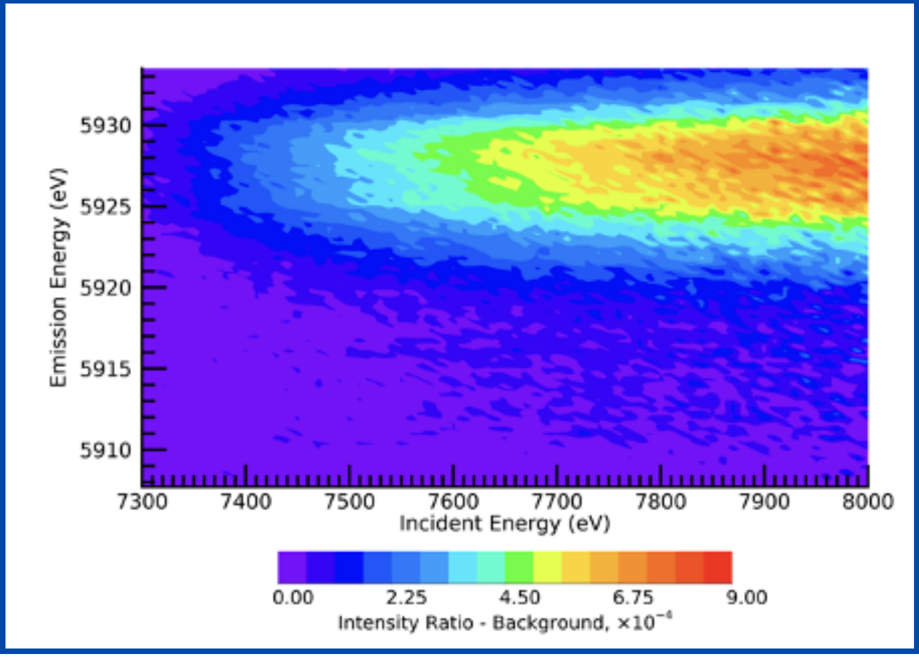

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Experimental: Chris Chantler, Zwi Barnea, Martin de Jonge [AS], Stephen Best, Ryan Trevorah, Martin Schalken, Ruwini Ekanayake, Geoff Cousland, Marcus John, Daniel Sier, Nich Tran, Alexis Illig, M N Kinnane, Justin A Kimpton, Lucas F Smale, D Paterson, A Payne

- La Trobe, Victoria: Chanh Q Tran, Tony Kirk
- Diamond: Sofia Diaz-Moreno, J Fred W Mosselmans
- James Hester [ANSTO], Dudley Creagh [Canberra], Joel Brugger [Monash], Barbara Etschmann

Theory: Chris Chantler, Jay Bourke, Lucas Smale, Chris Witte, Andrew Hayward, John Lowe, Joni Pham, Truong Nguyen, Feng Wang, Hamish Melia, Jonathan Dean, Finn Jenssens, Paarangat Pushkarna, Rosemary Zielinski, Yves Joly [Grenoble]

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Some Highlights of this Conference: New Physics in Precision Atomic Experiments

- Earlier today: **Hamish Melia, atomic theory and experiment: MCHDF theory and experiment for Cu $K\alpha_{3,4}$**
- **Paul di Paschale [La Trobe: Quantum Interference for X-ray Optics: Phase and Amplitude]**

Posters:

Jonathan Dean [Measuring X-ray spectra of 3d transition metals to World-best accuracy & resolution], Jack Webster [CSIRO: Detectors for Mars], Prof Feng Wang [Quantum Chemistry]

Rosemary Zielinski [MCDHF for Zinc Kα]

Truong VB Nguyen [The LCG-Welton Method for the Lamb Shift and MCDHF]

New Opportunities in Fundamental Atomic Physics, Solid State Theory, Experiment and Synchrotron Science, including Discovery of new satellites using extended range HERFD

1. Measurement of plasmon-coupling

2. XERT for high resolution nanostructure of Zn from XAFS

3. Discovery of a new satellite in manganese using extended range High Energy Resolution Fluorescence Detection, XR-HERFD. Identification and characterisation of many-body processes will shed light on analytical approaches and structure observed in experimental techniques, and a new light on Mn.

POSTERA CRESCAM LAUDE

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Atomic and Solid State Physics Working Together

TOPIC 1: PLASMON COUPLING: IMFP MEASUREMENTS FROM XAFS

- Experiments using X-ray Extended Range Technique (XERT) – 100 times more accurate than standard XAFS

  * C. T. Chantler *Eur. Phys. J.* 169 147 (2009)

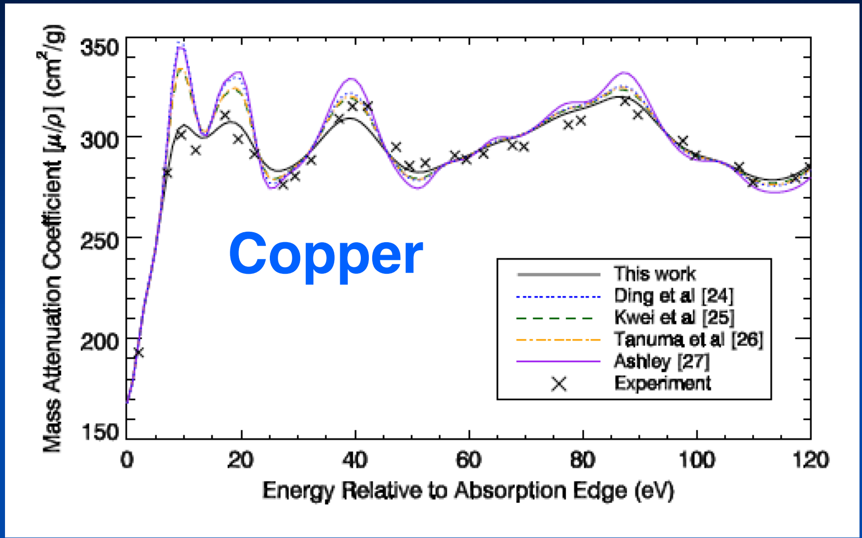
- New theory – FDMX – full-potential modelling over extended energy range - refined thermal parameters, core-hole relaxations and finite-cluster effects (FDMNES uses DFT LDA-U and TD-DFT)

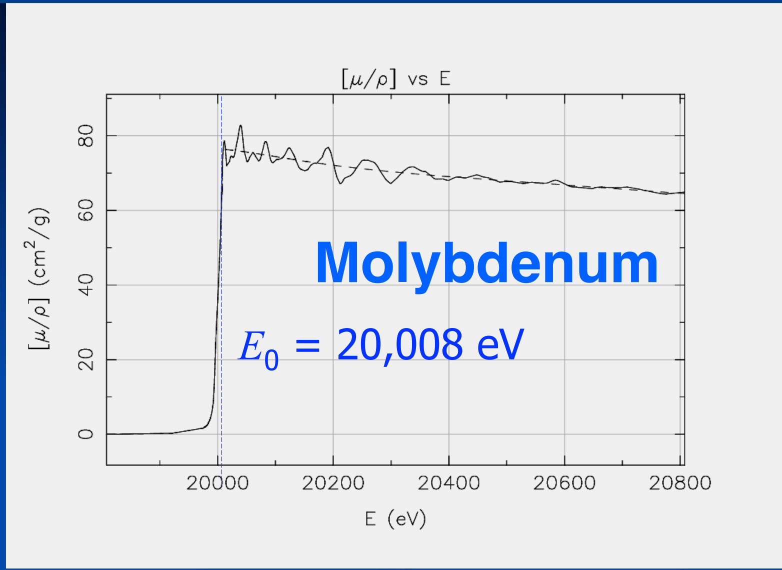
  * J.D Bourke et al. *Phys. Lett. A* 360 702 (2007)

  * JD Bourke, CT Chantler, *J Synch Rad* 23(2016)551-559

  * the advantage of theory simultaneously fitting XANES and XAFS [JD Bourke, CT Chantler, Y Joly: FDMX: Extended X-ray Absorption Fine Structure Calculations Using the Finite Difference Method, *J Synchrotron Radiation* 23 551-559 (2016)]

Measurement of plasmon-coupling

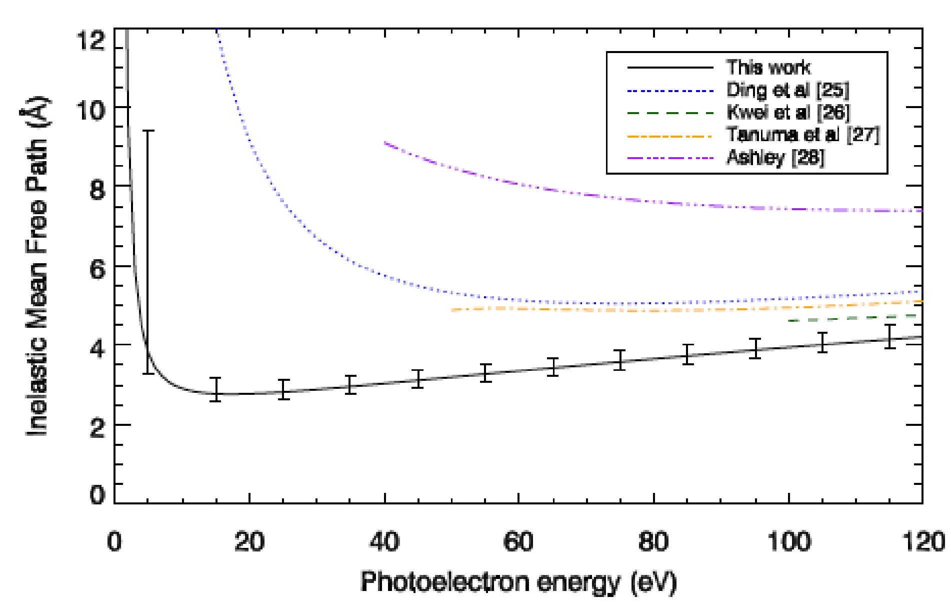




Mass Attenuation Coefficients (solid)
(error bars smaller than linewidth)

- CQ Tran, CT Chantler, Z Barnea, Physical Review Letts 90 (2003) 257401-1-4
- MD de Jonge, CQ Tran, CT Chantler, Z Barnea, BB Dhal, DJ Cookson, W-K Lee, A Mashayekhi, Phys. Rev. A 71, 032702 (2005) 032702-1-16
- JD Bourke, CT Chantler, Measurements of Electron Inelastic Mean Free Paths in Materials, Phys. Rev. Letters 104 (2010) 206601-1-4
- CT Chantler, JD Bourke, X-ray Spectroscopic Measurement of the Photoelectron Inelastic Mean Free Paths in Molybdenum, Journal of Physical Chemistry Letters 1 (2010) 2422-2427

Measurement of plasmon-coupling



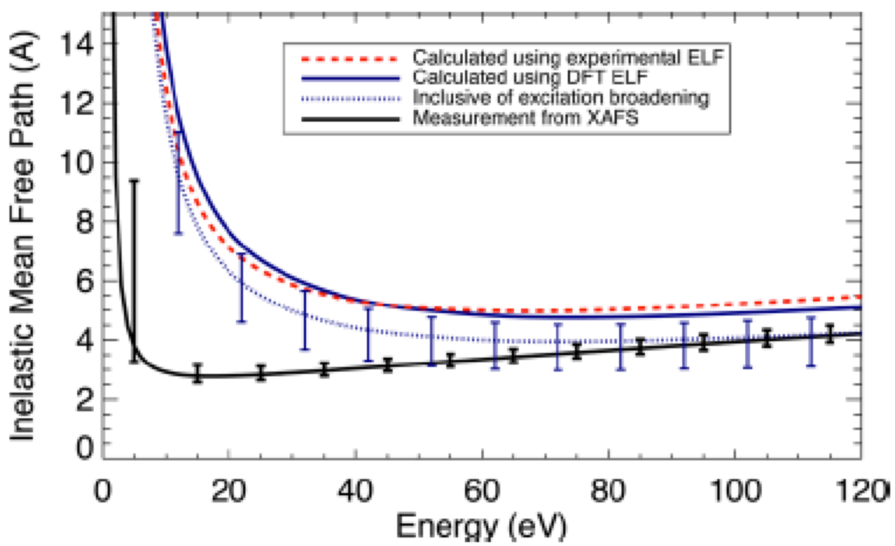


Figure 4. Electron inelastic mean free paths of copper calculated using theoretical optical loss data (solid blue curve) and measured optical loss data from Hagemann et al. (dashed red curve) compared with recent measurements using high-accuracy XAFS spectroscopy (black).[7] Also shown is a result inclusive of plasmon broadening quantified via a previous analysis of copper IMFPs (dotted blue curve),[14] along with a maximum-variational confidence interval.

er

MEASUREMENT OF PLASMON-COUPLING

- NEW Plasmon coupling theory (2014) – calculate γ using the loss spectrum itself

$$\lambda(E)_N^{-1} = \frac{\hbar}{a_o \pi E} \int_0^{\frac{E-E_F}{\hbar}} \int_{q_-}^{q_+} \int_0^{\infty} \frac{2}{\pi} \frac{\omega'}{q} \times \mathrm{Im}\left[\frac{-1}{\epsilon_{\mathrm{data}}(0,\omega')}\right] \times \mathrm{Im}\left[\frac{-1}{\epsilon_M(q,\omega,\gamma_i(q)_{N-1};\omega_p=\omega_i)}\right] d\omega' dq d\omega$$

$$\gamma_i(q)_N = \hbar \left.\frac{d\omega_q}{dq}\right|_{\omega_q,q} \lambda(E)_N^{-1}\Theta(N-\delta)$$

* JD Bourke, CT Chantler *J. Phys. Chem. Lett.* 6 (2015) 314-319

- First physical, uniquely constrained optical data model since the Penn algorithm [1987]
- Self consistent from successive iterations – broadening comes from coupling between excitation channels

Measurement of plasmon-coupling

RESULTS FOR MOLYBDENUM

- Broadening contributes a substantial reduction in IMFP from a fully lossless Lindhard model
- The reduction has a strong impact from excitations below the plasma frequency

•Agreement with experiment is improved greatly across all energies

- New predictions for low energy electron transport in any matter. Major differences below 200 - 300 eV, LEED, EELS, Monte Carlo, detector design

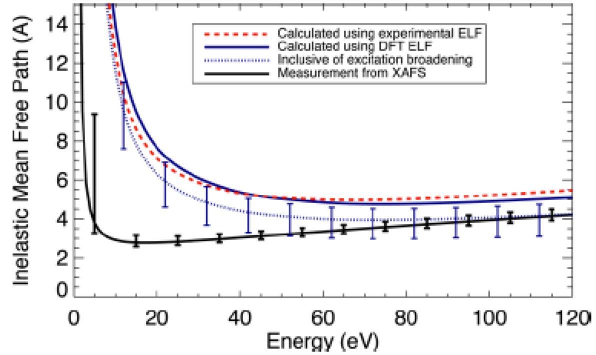
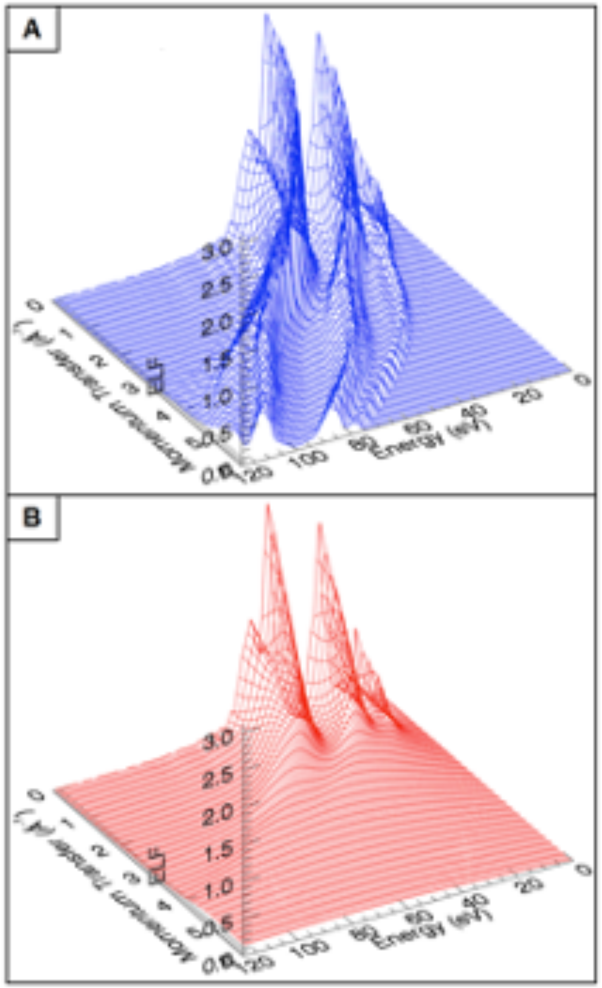


Figure 4. Electron inelastic mean free paths of copper calculated using theoretical optical loss data (solid blue curve) and measured optical loss data from Hagemann et al. (dashed red curve) compared with recent measurements using high-accuracy XAFS spectroscopy (black).[7] Also shown is a result inclusive of plasmon broadening quantified via a previous analysis of copper IMFPs (dotted blue curve),[14] along with a maximum-variational confidence interval.

Bourke, Chantler J Phys Chem A 118 (2014) 909

C T Chantler, J D Bourke, Low-energy electron properties: Electron inelastic mean free path, energy loss function and the dielectric function. Rece the plasmon-coupling theory. Ultramicroscopy 201 Mar (2019) 38-48

MEASUREMENT OF PLASMON-COUPLING



The electron energy loss function (ELF) of Mo. (A) is calculated using a lossless Lindhard type model, while (B) utilises a self-consistent coupled-plasmon model.

C T Chantler, J D Bourke, Low-energy electron properties: Electron inelastic mean free path, energy loss function and the dielectric function Recent measurement and the plasmon-coupling theory, Ultramicroscopy 201 Mar (2019) 38-48

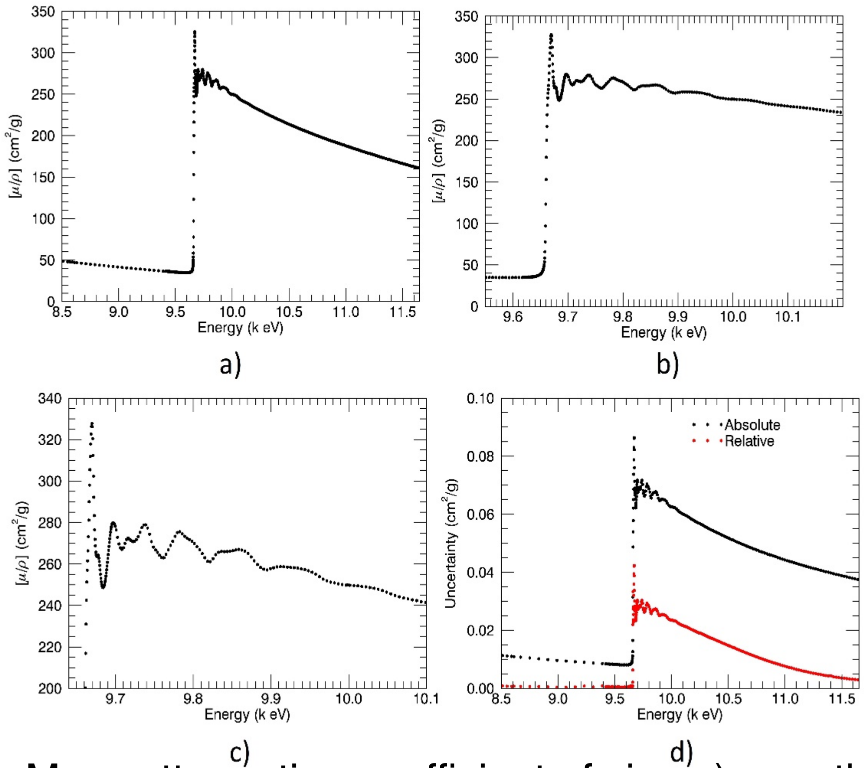
Topic 2: High accuracy mass attenuation coefficients, and X-ray absorption spectroscopy of Zinc – The first X-ray Extended Range Technique experiment in Australia

Mass attenuation coefficients and EXAFS

R S K Ekanayake, C T Chantler, D Sier, M J Schalken, A J Illig, M D de Jonge, B Johannesen, P Kappen, C Q Tran, High accuracy mass attenuation coefficients, and X-ray absorption spectroscopy of zinc – the first X-ray Extended Range Technique-like experiment in Australia, J Synch Rad 28(5) (2021) 1476-1491

R S K Ekanayake, C T Chantler, D Sier, M J Schalken, A J Illig, M D de Jonge, B Johannesen, P Kappen, C Q Tran, High accuracy measurement of mass attenuation coefficients and the imaginary component of the atomic form factor of zinc from 8.51 keV to 11.59 keV, and X-ray absorption fine structure with investigation of zinc theory and nanostructure J Synch Rad 28(5) (2021) 1492-1503

D Sier, R S K Ekanayake, C T Chantler, The Significance of Fluorescent Scattering in Transmission X-ray absorption spectroscopy and X-ray absorption fine structure X-Ray Spectrometry 51 (2022) 91-100 doi 10.1002/xrs.3262



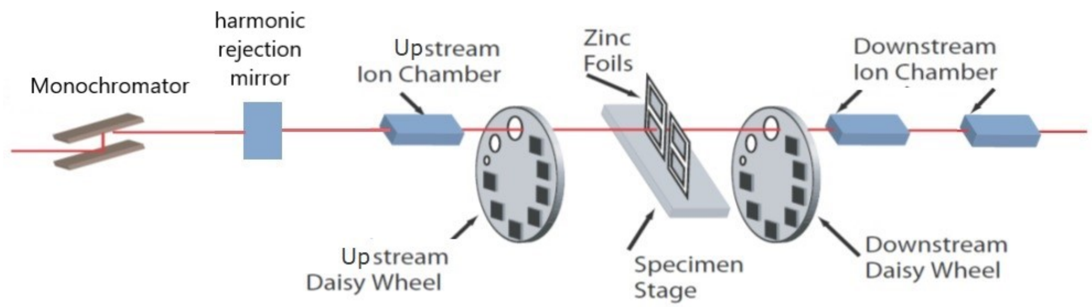
$$\left[\frac{\mu}{\rho}\right] \text{abs} = 34.765 - 327.760 \left(cm^2 g^{-1}\right)$$

$$\sigma_{abs} = 0.023\% - 0.0357\%$$

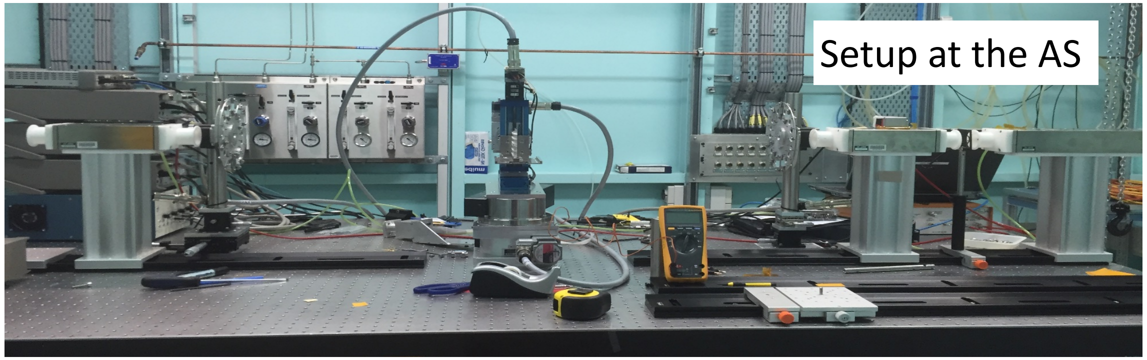
$$\sigma_{rel} = 0.000677\% - 0.027\%$$

Mass attenuation coefficient of zinc a) over the energy range of 8.51 keV to 11.59 keV; b) covering the edge and XAFS region; c) in the central XAFS region; and d) absolute and relative percentage uncertainties.

Experiment: X-ray Extended Range Technique at the Australian Synchrotron



X-ray Extended Range Technique (XERT) experimental setup [13] for collecting XAFS data of Zn (10 µm, 25 µm & 50 µm) **at room T**



Energies:
from 8.51 keV to 11.59 keV

Beam spot size 2.4mmx0.4mm

Ekanayake, RSK *et al. J Synchrotron Rad*, 28, (2021), 1476-1491

XERT and AS: Zn nanostructure from XAS

Structural Parameters

Parameter	Value	s.e.	Parameter	Value	s.e.
ΔE_0 (eV)	4.70	0.29	α_3 ***	1.0061	0.0013
S_0^2	0.904	0.037	σ_1^2 * (Å^2)	0.0101	0.0003
Zn-Zn *(Å)	2.660	0.003	σ_2^2 ** (Å^2)	0.0198	0.0008
Zn-Zn **(Å)	2.832	0.008	σ_3^2 *** (Å^2)	0.0221	0.0007
α_1 *	0.9999	0.0010	σ_3^2 **** (Å^2)	0.0169	0.0008
α_2 **	0.9737	0.0027	$\Delta\chi_r^2$	6.66	

X-ray diffraction data [16]

Zn-Zn * =2.6636(1) (Å)
Zn-Zn **= 2.9120(1) (Å)

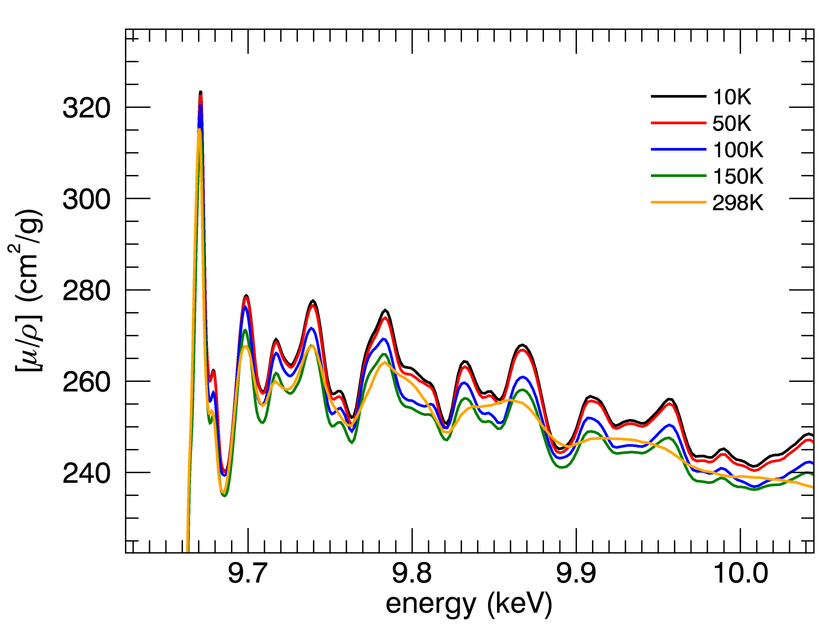
* for nearest neighbour (shortest) scattering path.
* * for the second nearest atom.
* ** most other scattering paths.
* *** for single scattering paths 8 and 9.

- Our bond lengths are 0.1%(±0.10%) and 2.7%(±0.3%) smaller respectively.
- The scaling parameter obtained for the other bond lengths are 0.62%±0.13% larger than the scaling of the nearest neighbour bond length
- This 5-7 standard error variations can be due to dynamic motion, or to the path-length including motion perpendicular to the bond length.
- **This suggests dynamic motion in the crystal lattice inaccessible by other techniques.**

Uncertainties in fitting analysis returns nanostructure and bonding even to 0.1% and to 0.3 picometres

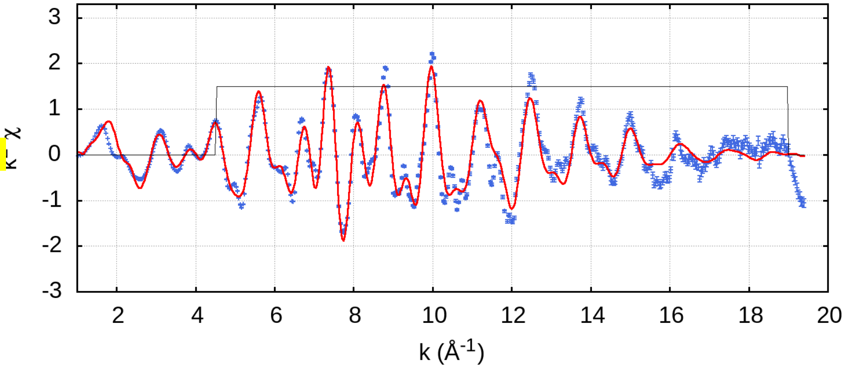
Ekanayake, RSK *et al. J Synchrotron Rad*, 28, (2021), 1492-1503, 16. Nuss *et al., Z. Anorg. Allg. Chem.*,636, (2010), 309-313

Evolution of Zinc Nanostructure from 10K to Room Temperature – The First Hybrid Experiment in Australia

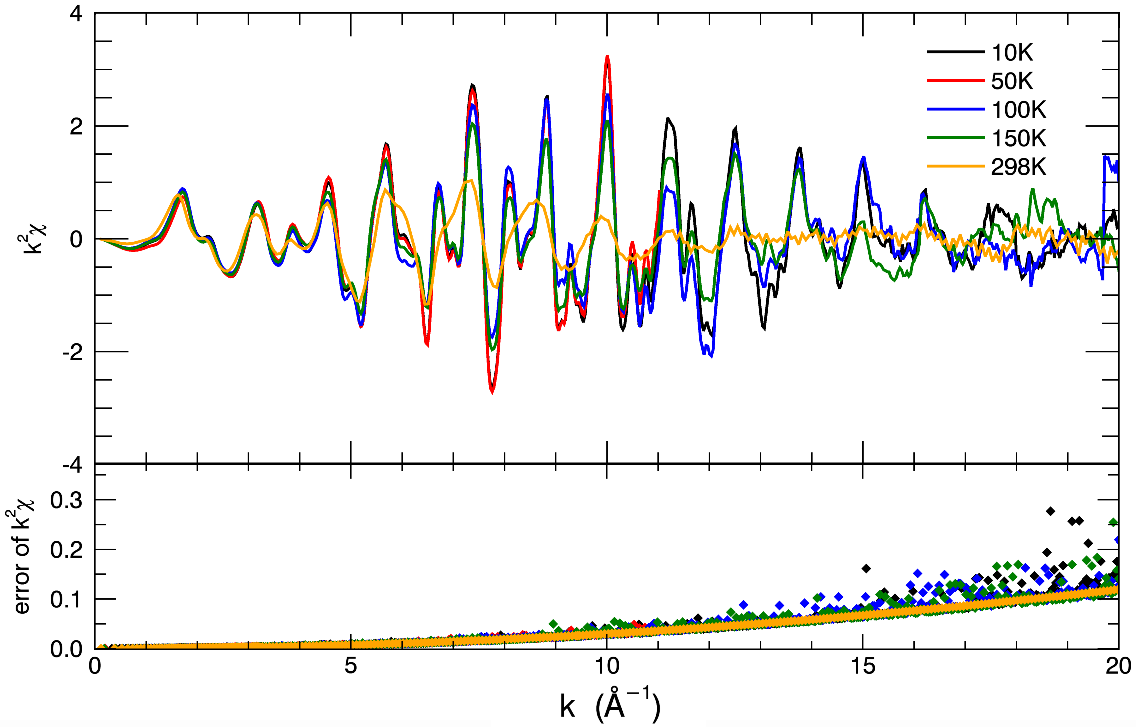


Marcus W John, Daniel Sier, Ruwini S K Ekanayake, Martin J Schalken, Chanh Q Tran, Bernt Johannessen, Martin D de Jonge, Peter Kappen, C T Chantler, High accuracy transmission and fluorescence XAFS of zinc at 10 K, 50 K, 100 K and 150 K using the Hybrid technique J Synchrotron Radiation 30 (2023) doi 10.1107/S1600577522010293

- The first data acquired with the Hybrid technique in Australia
- The first data set of mass attenuation coefficients for transition metals over a wide temperature series to low temperatures [10K].
- The first simultaneous measurement of transmission and fluorescence XAS on ideal systems for high accuracy with meaningful comparisons.
- Improve methods for correcting self-absorption effects and anomalies in fluorescence spectrometry

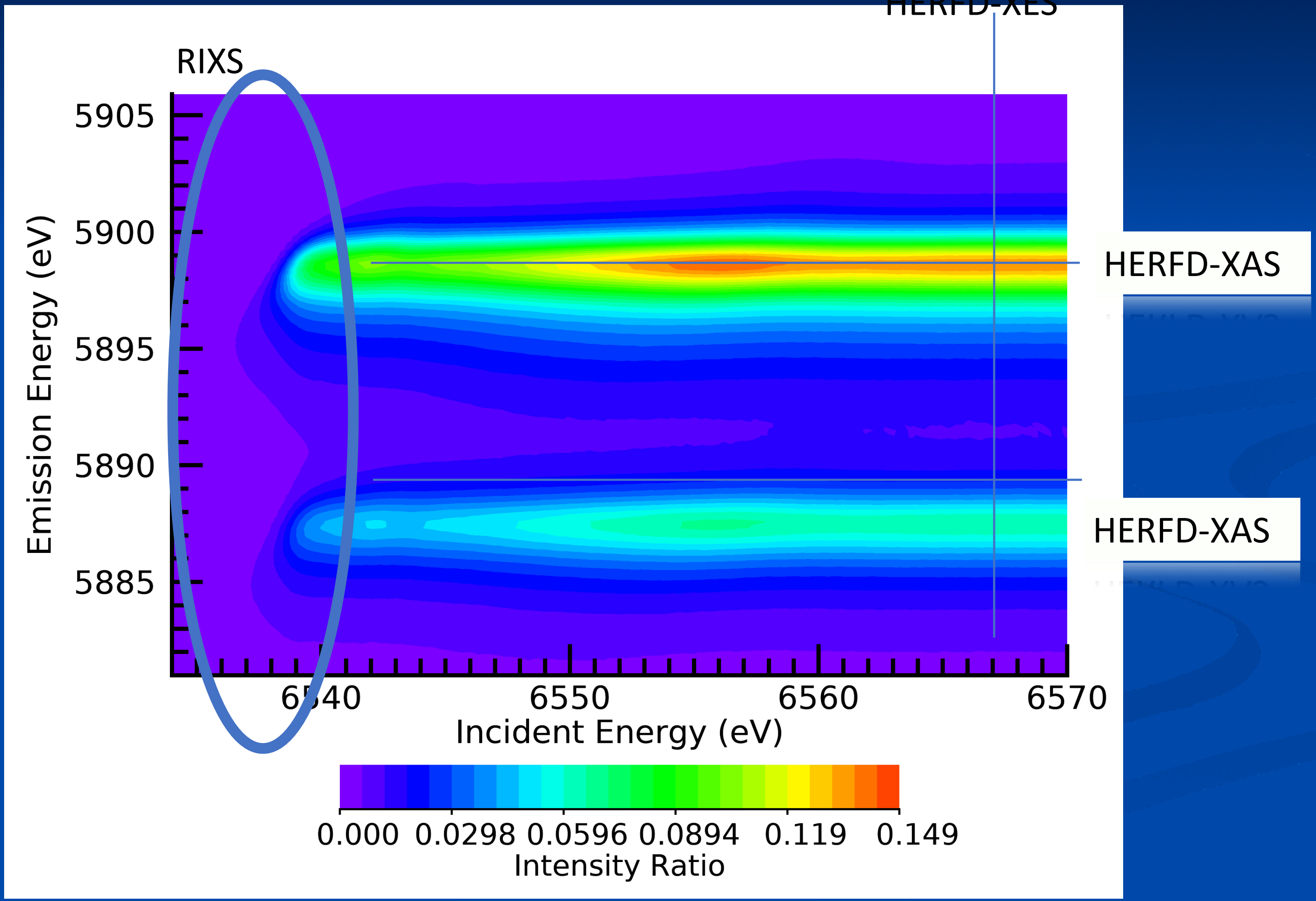


- $\left[\frac{\mu}{\rho}\right]$ for low temperature Zinc accurate to 0.03% for transmission and 0.18% for fluorescence spectroscopy. Previous estimated accuracies are 1% - 5%.
- A new method for determining anisotropic thermal expansion accurate to 0.65%
- Evolution of thermal properties in Zinc



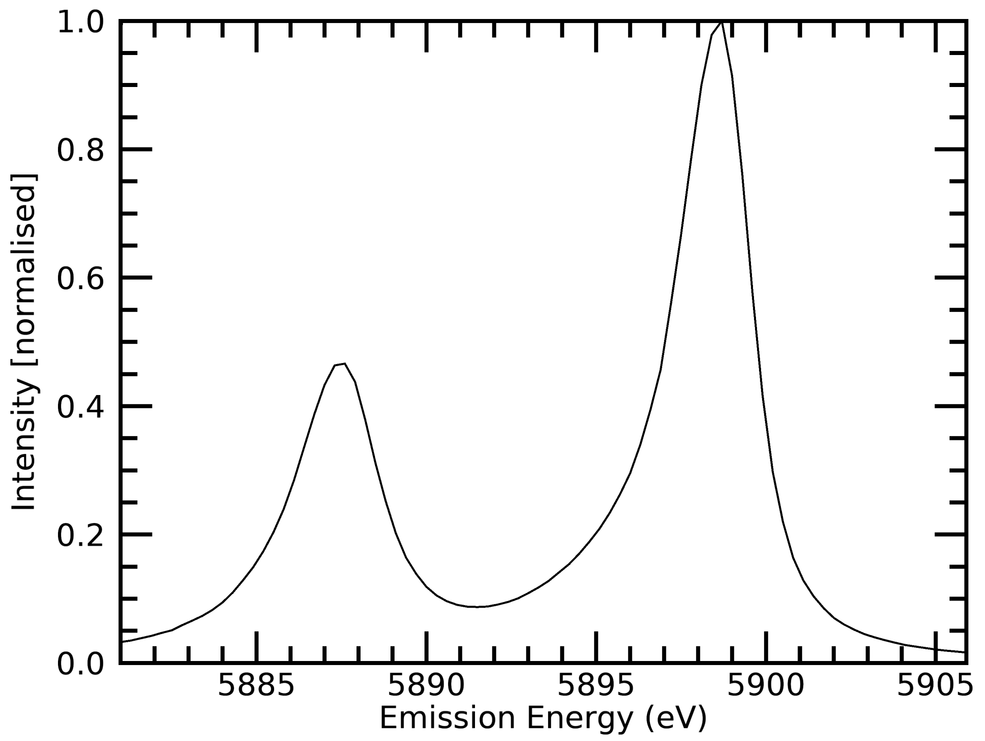
Topic 3.Discovery of a new satellite in manganese using extended range High Energy Resolution Fluorescence Detection, XR-HERFD.

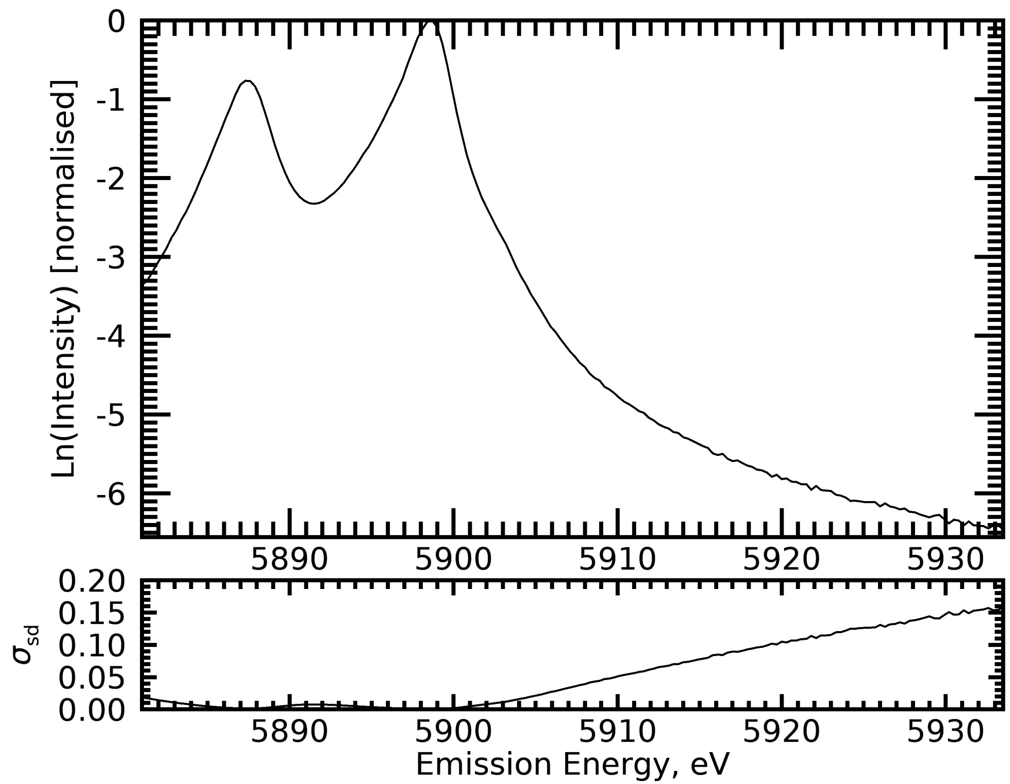
RIXS, HERFD data circa 2000 to 2021



X-ray Spectroscopy - Advances

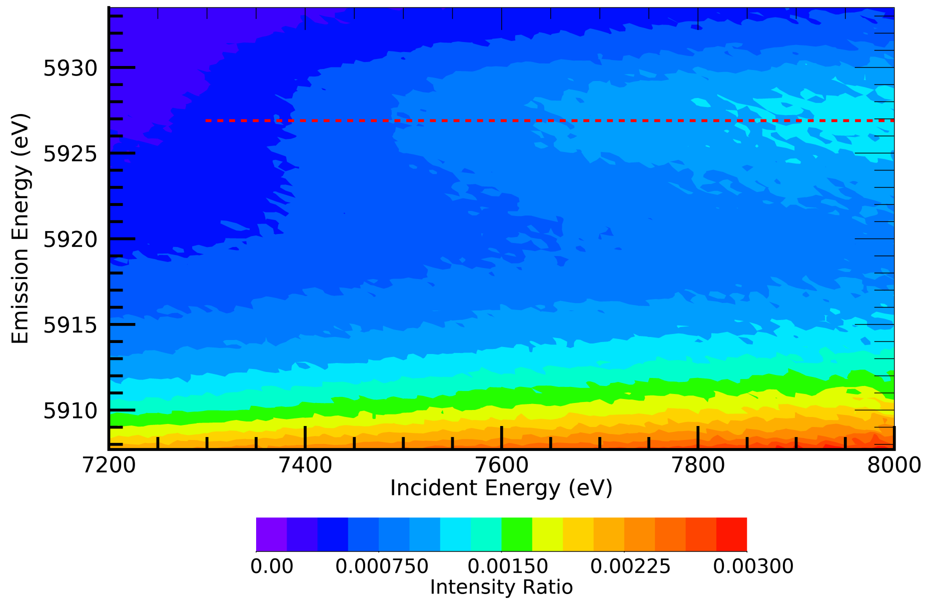
HERFD data Chantler et al. 2021





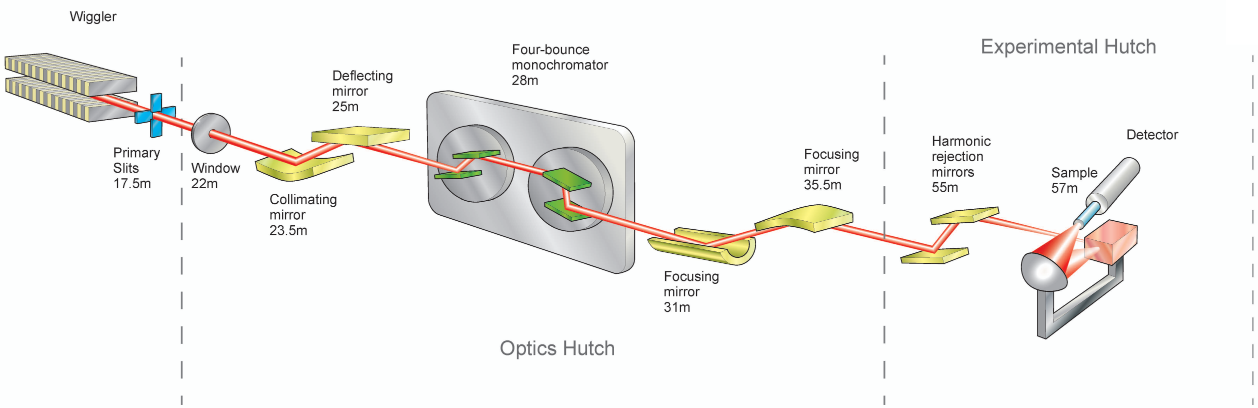
X-ray Spectroscopy - Advances HERFD data Chantler et al. 2021

Q: When is a characteristic Kα XES spectrum not 1s-2p?



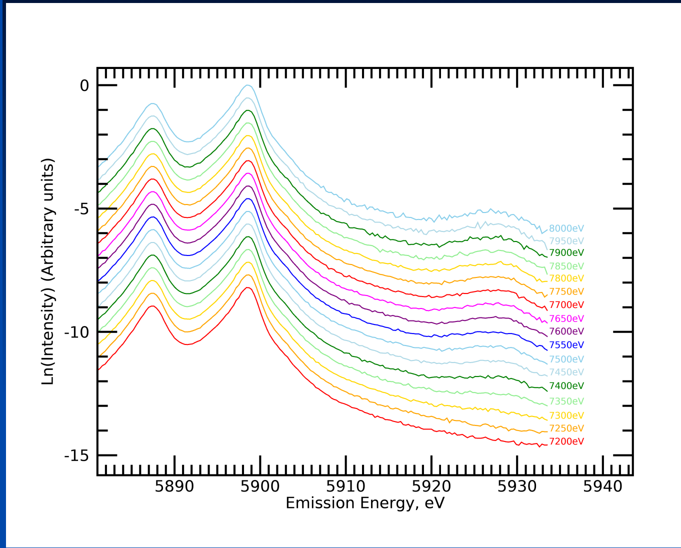
I20 Branch line

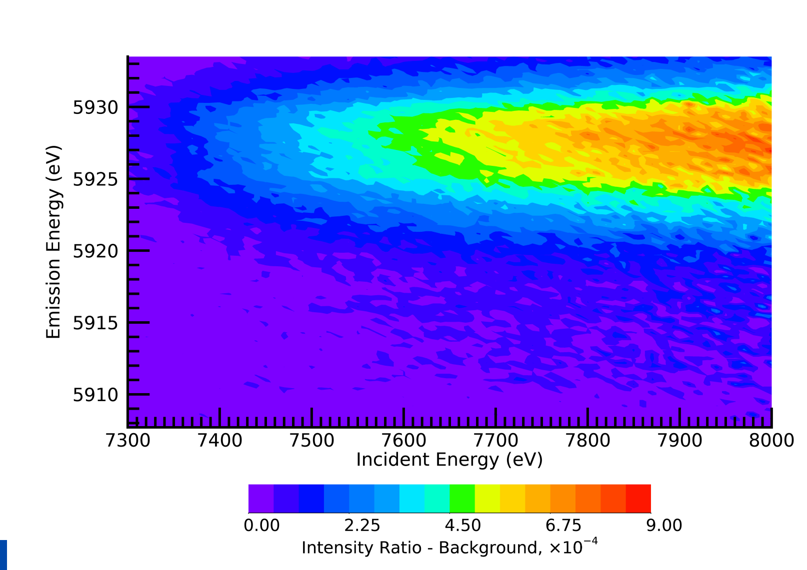
I20 Scanning Branch Diamond March 2021
eXtended-Range HERFD, XAS-XES

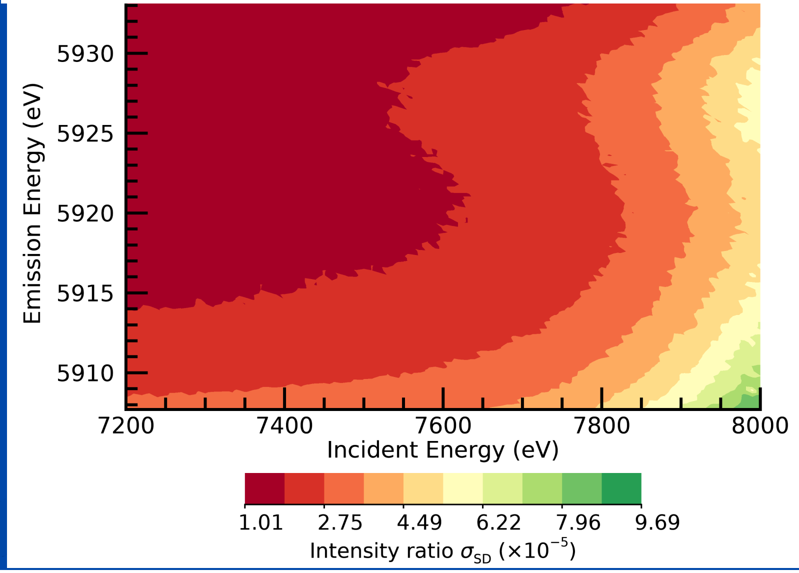


X-ray Spectroscopy - Advances

HERFD data Chantler et al. 2021

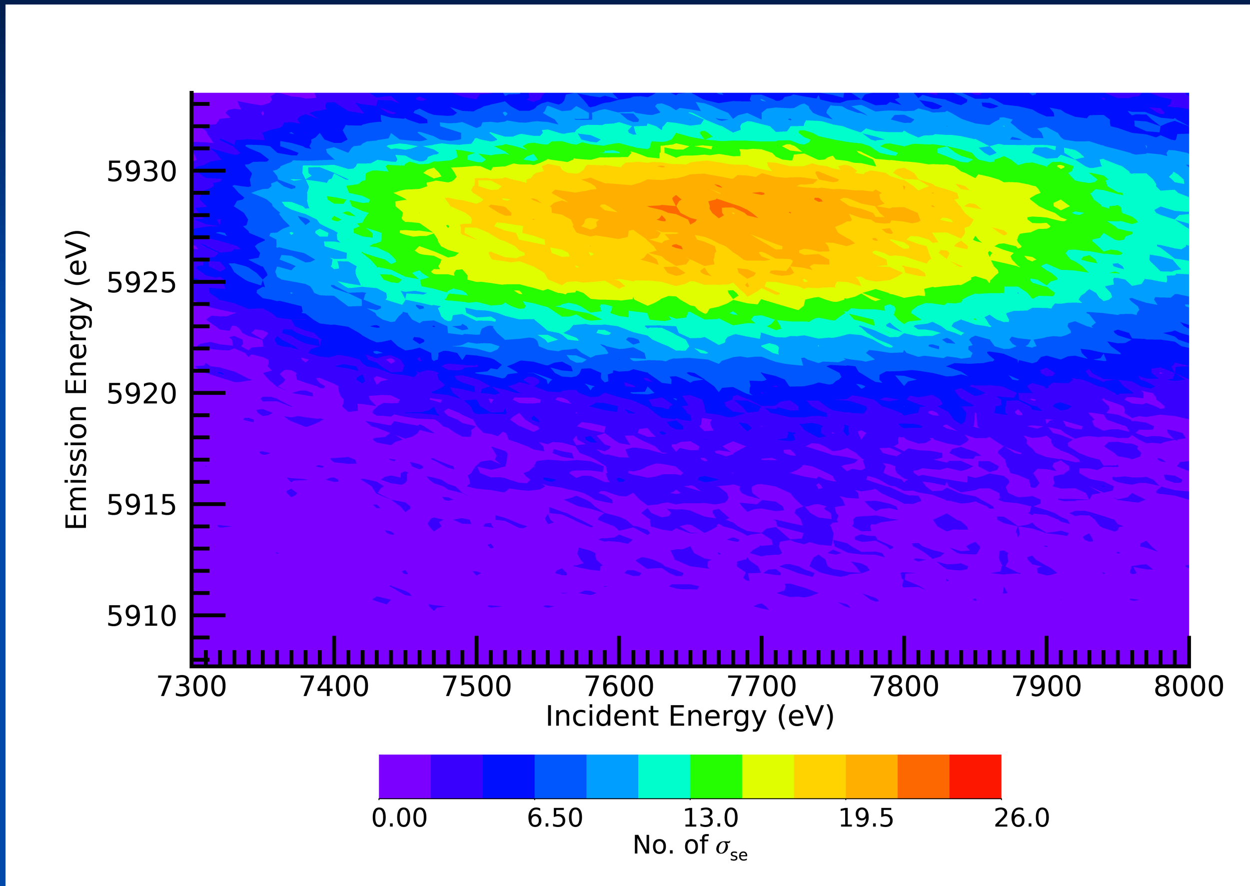






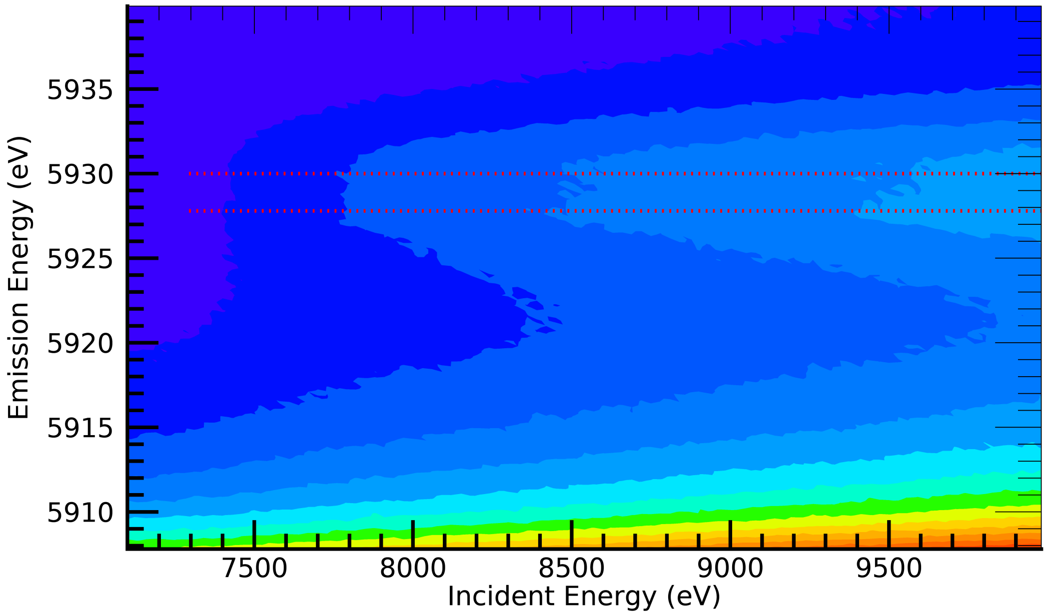
X-ray Spectroscopy - Advances

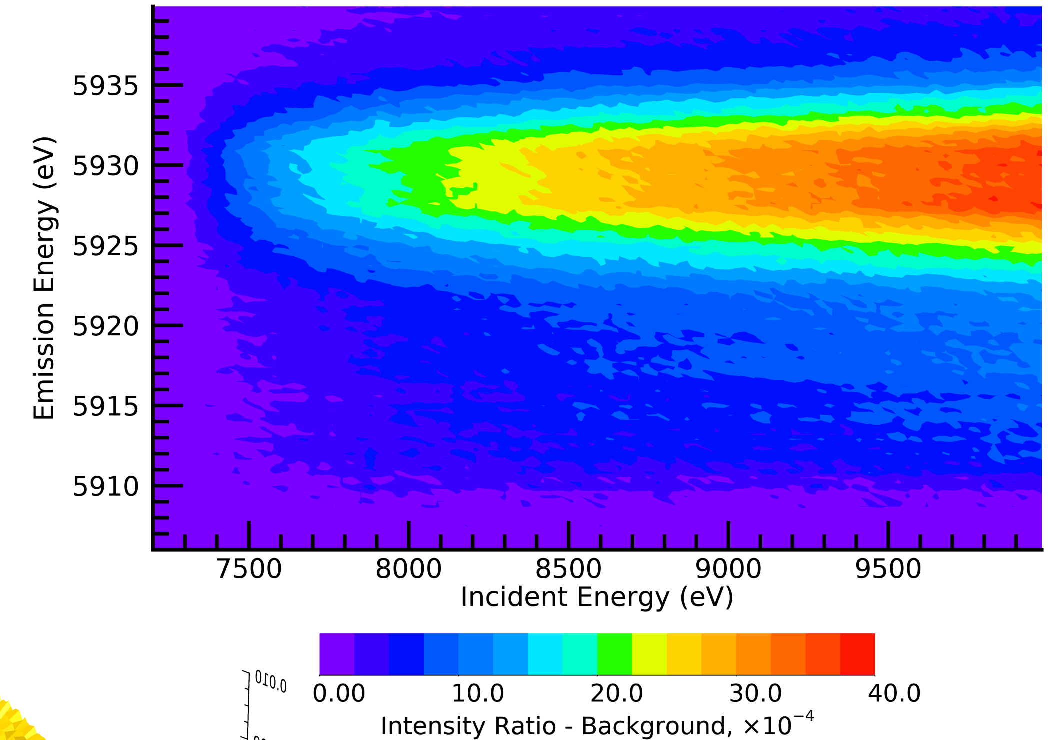
HERFD data Chantler et al. 2021

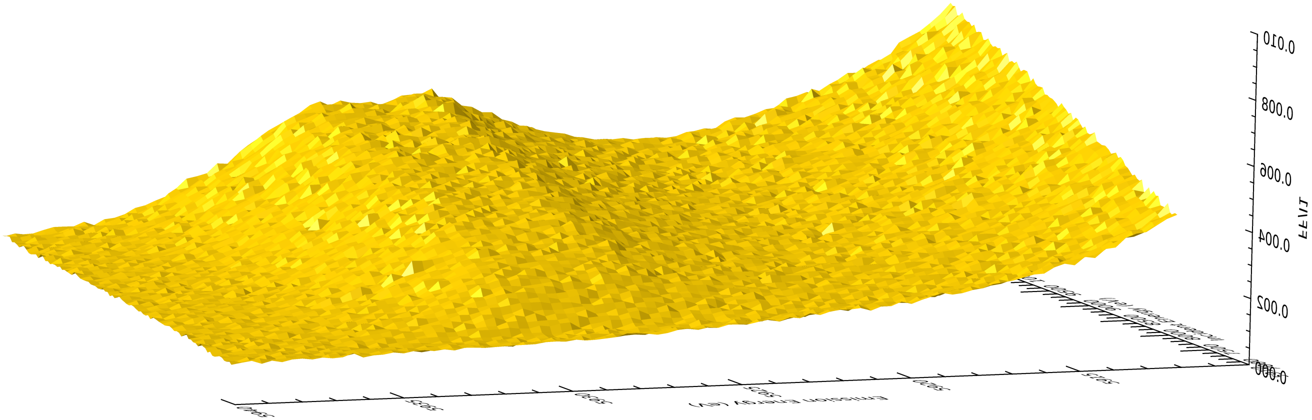


Discovery: >10 standard error significance at every data point!

X-ray Spectroscopy - Advances HERFD data Chantler et al. Dec 2021







Characteristic spectra: A "Simple" Problem

Magnetic Interactions

Correlation

Multiple Electrons

Finite Nuclear Size

Molecules

$$i\frac{\partial}{\partial t}\Psi = -\frac{1}{2}\nabla^2\Psi + V\Psi$$

QED

Vacuum Polarisation

Self Energy

Relativity

Open Shells

Characteristic spectra: A "Simple" Problem

Magnetic Interactions

Correlation

Multiple Electrons

Finite Nuclear Size

Molecules

$$i\frac{\partial}{\partial t}\Psi = \left(\beta c^2 + c\alpha \cdot p\right)\Psi$$

QED

Vacuum Polarisation

Self Energy

Relativity

Open Shells

Characteristic spectra: A "Simple" Problem

Magnetic Interactions

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Multiple Electrons

Finite Nuclear Size

Molecules

QED

$$i\frac{\partial}{\partial t}\Psi = \sum_{i}^{N}\left(\beta c^2 + c\alpha \cdot p\right)\psi + \sum_{i<j}^{N}\frac{1}{|r_i - r_j|}\psi$$

Vacuum Polarisation

Self Energy

Relativity

Open Shells

Characteristic spectra: A "Simple" Problem

Magnetic Interactions

Correlation

Multiple Electrons

Finite Nuclear Size

Molecules

QED

Vacuum Polarisation

Self Energy

Relativity

Open Shells

$$i\frac{\partial}{\partial t}\Psi = \sum_{i}^{N}\left(\beta c^2 + c\alpha\cdot p\right)\psi + \sum_{i<j}^{N}\left(\frac{1}{|r_i - r_j|}\right.$$

$$-\frac{\alpha_i\cdot\alpha_j}{|r_i - r_j|} - \frac{\alpha_i\cdot\alpha_j}{|r_i - r_j|}\left[cos\left(\frac{|\omega_i - \omega_j||r_i - r_j|}{c}\right) - 1\right]\psi$$

$$\left.+c^2(\alpha_i\cdot\nabla_i)(\alpha_j\cdot\nabla_j)\frac{cos\left(\frac{|\omega_i-\omega_j||r_i-r_j|}{c}\right) - 1}{|\omega_i - \omega_j|^2|r_i - r_j|}\right)$$

Characteristic spectra: A ~~"Simple"~~ Problem

Magnetic Interactions

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Relativity

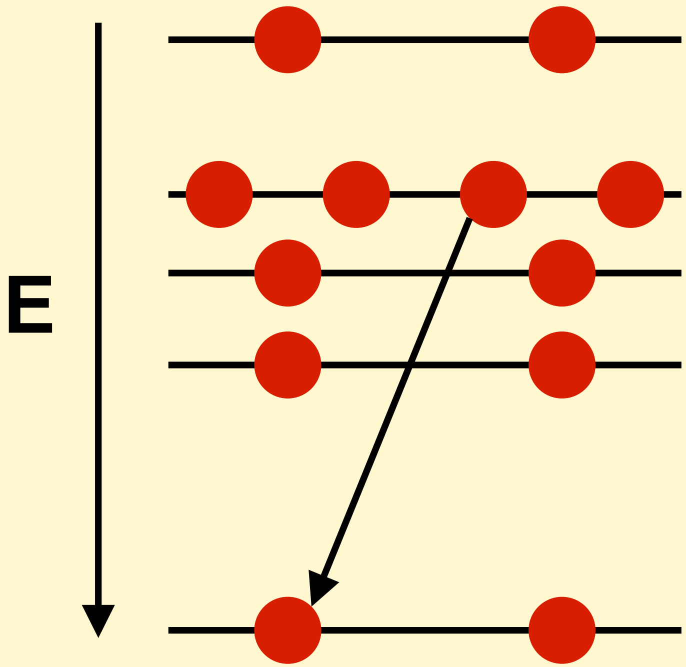
Open Shells

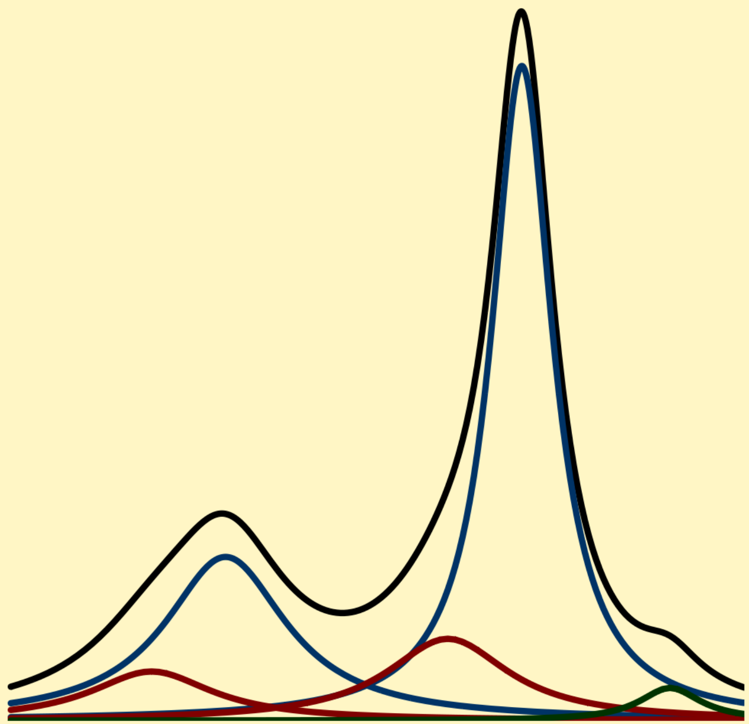
$$i\frac{\partial}{\partial t}\Psi = \sum_{i}^{N}\left(\beta c^2 + c\alpha\cdot p\right)\psi + \sum_{i<j}^{N}\left(\frac{1}{|r_i - r_j|}\right.$$

$$-\frac{\alpha_i\cdot\alpha_j}{|r_i - r_j|} - \frac{\alpha_i\cdot\alpha_j}{|r_i - r_j|}\left[cos\left(\frac{|\omega_i-\omega_j||r_i-r_j|}{c}\right) - 1\right]\psi$$

$$\left. + c^2(\alpha_i\cdot\nabla_i)(\alpha_j\cdot\nabla_j)\frac{cos\left(\frac{|\omega_i-\omega_j||r_i-r_j|}{c}\right) - 1}{|\omega_i-\omega_j|^2|r_i-r_j|}\right)$$

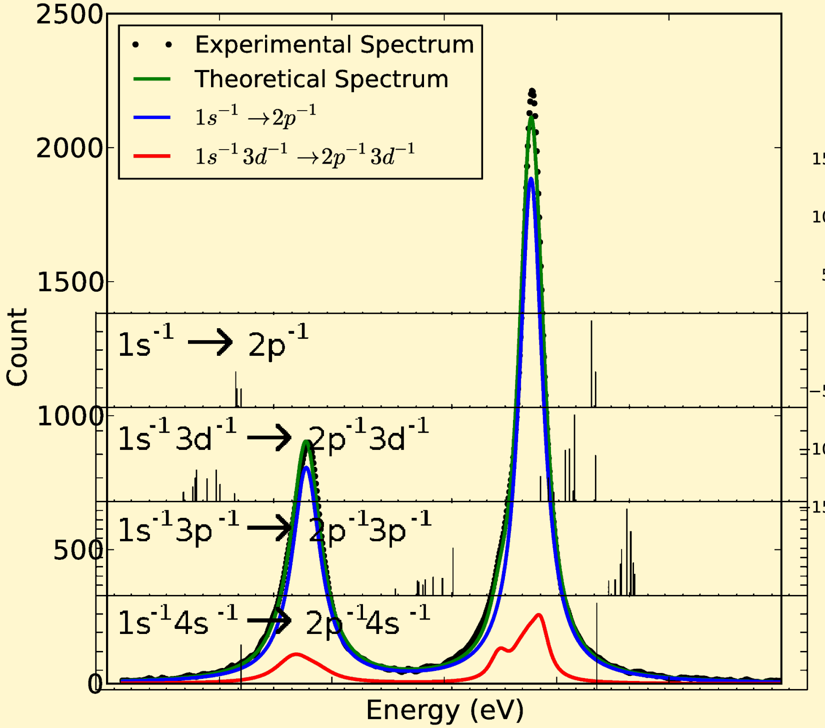
The Kα Spectrum

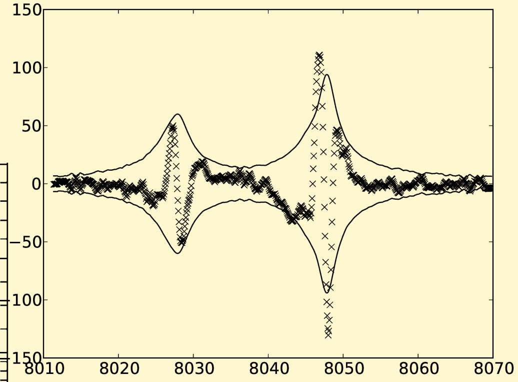




X-ray Spectroscopy - Advances

Copper Kα Photoemission Spectrum





Experimental Data: Deutsch et al., Phys. Rev. A., 51: 283, (1995)

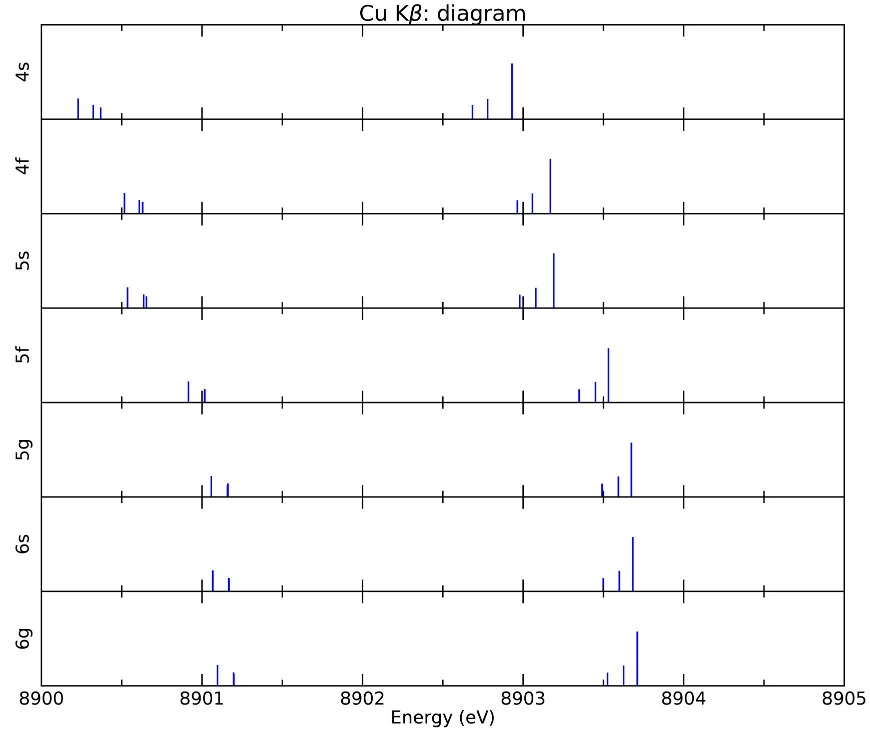
C. T. Chantler, J. A. Lowe, I. P. Grant. *Phys. Rev. A.*, 82:052505, (2010)

J. A. Lowe, C. T. Chantler, I. P. Grant. Phys. Rev. A., 83:060501, (2011)

C. T. Chantler, J. A. Lowe, I. P. Grant. *Phys. Rev. A.*, 85: 032513, (2012)

A new process … not 1s - 2p in the characteristic spectrum

- **New theory can now see the 100-1000 spectral components of characteristic X-ray radiation for X-ray spectroscopy and fundamental processes**
- Multiconfiguration Dirac-Hartree-Fock (MCDHF). Diagram spectra expanded to 5s with simultaneous convergence of 28000 configuration state functions (CSFs), Kα, and to 6g with simultaneous convergence of 91000 CSFs, Kβ, eigenvalue convergence to ±0.03 eV or 0.00025%, 10x improved upon past work.
- Biorthogonalisation, developments of the active space approach, analysis of markers for theoretical convergence of eigenvalues, and the question of self-consistency for Kα and Kβ.
- Gauge convergence, eigenvalue convergence, A-coefficient convergence. Without the satellite spectra it is not possible to make use of the increased accuracy of the diagram computations.
- Cu Kα $3d^8$ double-shake satellite spectrum: 1506 unique eigenvalues (transitions); simultaneous convergence of 593 000 CSFs
- T V B Nguyen, H A Melia, Finn I Janssen, C T Chantler, Theory of Copper Kα and Kβ Diagram Lines, Satellite Spectra, and ab initio Determination of Single and Double Shake Probabilities



A new process … not 1s - 2p in the characteristic spectrum

- **New theory can now see the 100-1000 spectral components of characteristic X-ray radiation for X-ray spectroscopy and fundamental processes**
- Multiconfiguration Dirac-Hartree-Fock (MCDHF). Diagram spectra expanded to 5s with simultaneous convergence of 28000 configuration state functions (CSFs), Kα, and to 6g with simultaneous convergence of 91000 CSFs, Kβ, eigenvalue convergence to ±0.03 eV or 0.00025%, 10x improved upon past work.
- Biorthogonalisation, developments of the active space approach, analysis of markers for theoretical convergence of eigenvalues, and the question of self-consistency for Kα and Kβ.
- Gauge convergence, eigenvalue convergence, A-coefficient convergence. Without the satellite spectra it is not possible to make use of the increased accuracy of the diagram computations.
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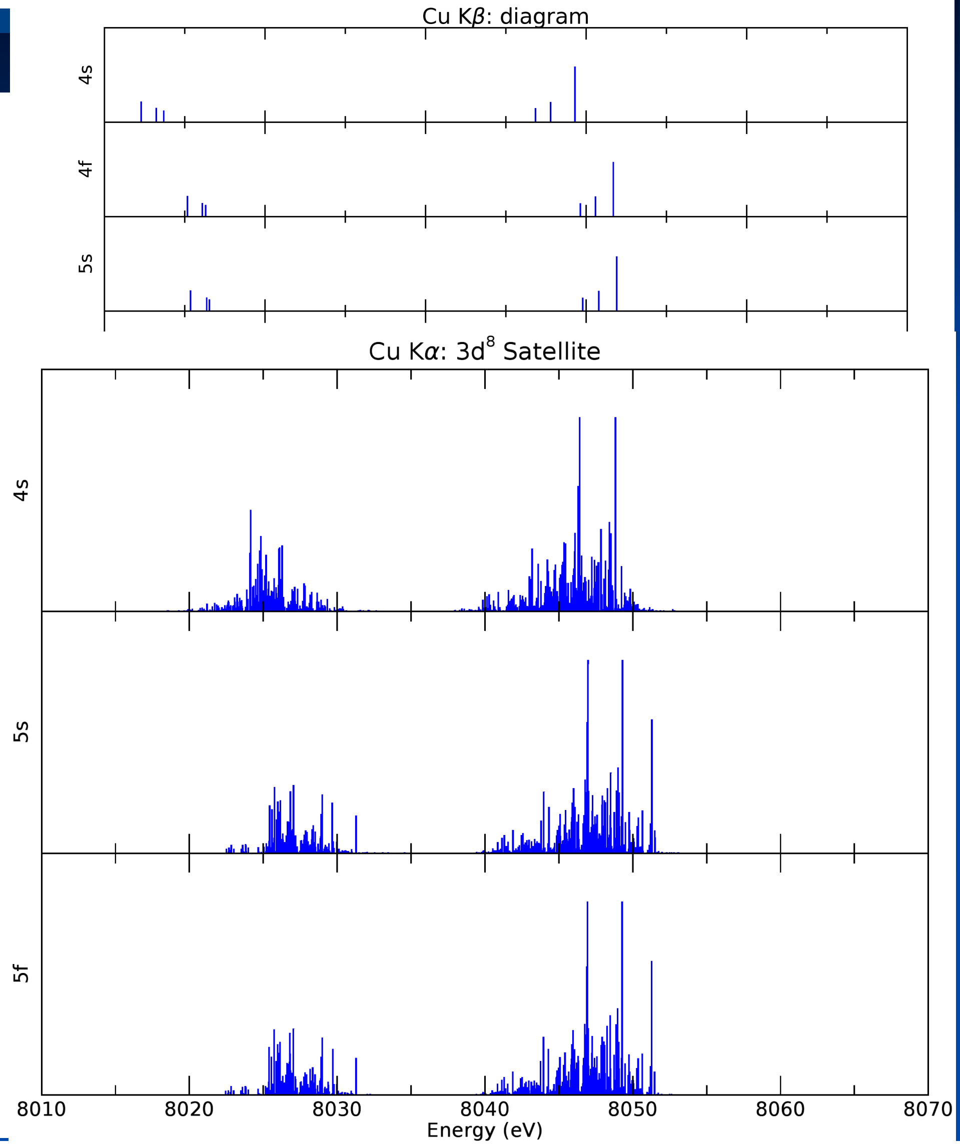
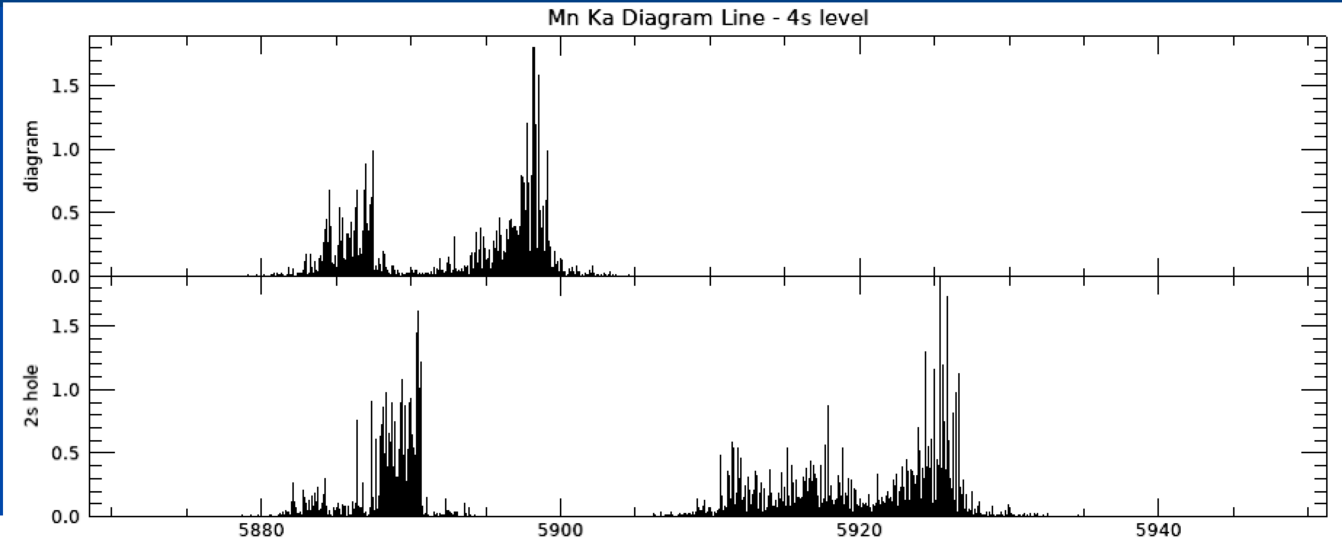
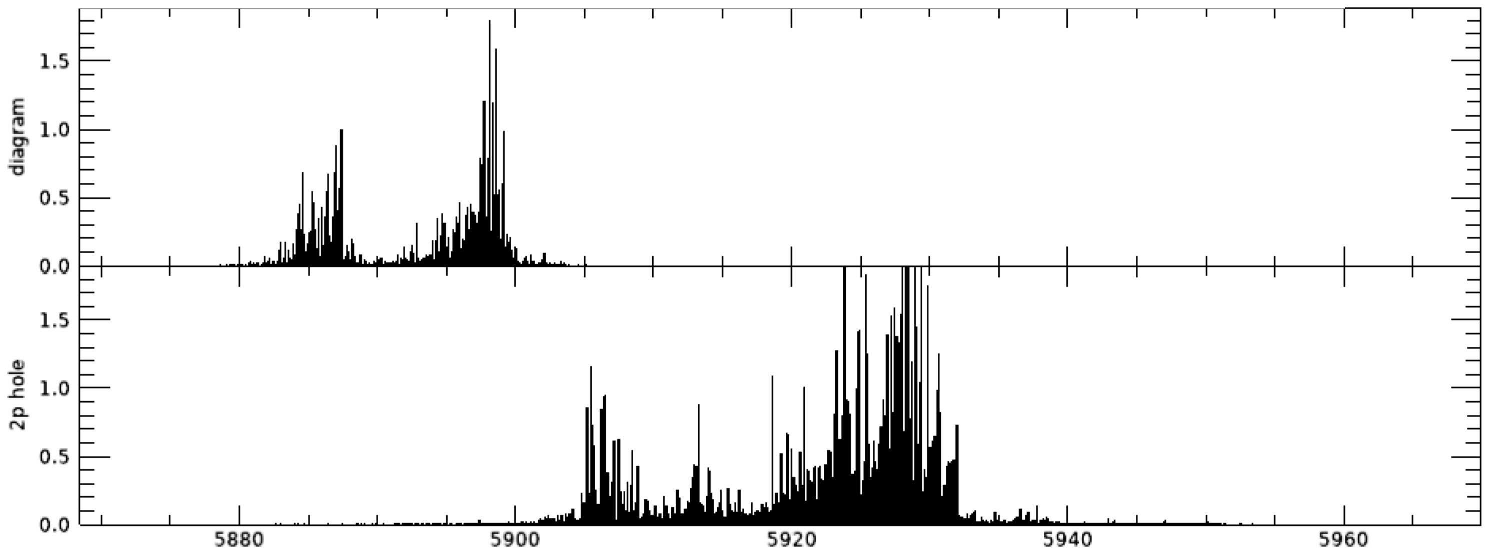


Not 1s-2p … advanced solid state physics





Current excitement: Consequences:

Identification and characterisation of these many-body processes can shed light on the XAFS spectra and how to interpret them, and hence how to measure the dynamical nanostructure observable with these technologies.

This is the first study of XES to observe these processes.

We report the discovery of a new satellite in manganese

using our newly developed technique, which we call extended range High Energy Resolution Fluorescence Detection, XR-HERFD

It explains and measures what used to be hidden inside the data and assumed to be an empirical fitting constant.

This applies to physics, chemistry, and biology for RIXS, HERFD and general XAS and XES studies, especially by explaining a series of anomalies in the data and theory, and permitting accurate nanostructural determination.

Many-body transitions are a bane, or major challenge, of current advanced theory and modelling of XAFS and related technologies such as RIXS and HERFD, especially because these are hard to compute in any density functional theory including time-dependent DFT. A core reason for this theoretical challenge is the electron correlation, which for complex open-shell atomic or molecular or solid-state theory are major open questions with ill-defined approaches. Indeed, this remains true even for purely atomic relativistic theory. However, here we can *see* them and *measure* them for the first time, including far from the high-energy impact approximation limit.

Current excitement: Consequences:

XAFS, whether for transmission or fluorescence experiments, or even high-resolution HERFD-XAS spectra, is currently modelled with a key (fitting) parameter S_0^2, the 'many body reduction factor' which is stated to represent the loss of correlation and signal of the quantum interference of the photoelectron wave due to many-body processes – exactly as we observe explicitly in this experiment.

However, as such, S_0^2 is often fixed to a convenient value e.g. 0.9, 0.8 or something in sympathy with naïve estimates; or is empirically fitted across the fitting range of the photoelectron quantum interference in energy or wavevector *k*-range. This parameter as a fitted or fixed variable, is 100% correlated with the coordination number, so if we do not know S_0^2 then the uncertainty in the coordination number increases. Understanding or defining this removes significant correlation uncertainty in the coordination number.

Our data and result proves that S_0^2 can in fact now be directly investigated – and that we see it change with energy. Hence, we prove that S_0^2 is energy- and wavevector-dependent. From the figures, it is clear that S_0^2 depends upon the integration range and resolution of the optics and detector system; and that it should decrease with increasing energy

This new peak is an *n=2* satellite spectrum and a shake-off many-body process. It may be the *2p* satellite spectrum to the diagram *1s-2p* fluorescence spectrum. If so, it represents a transition from the hole state Mn $1s^{-1}2p^{-1}$ to $2p^{-2}$, or $1s2s^2 2p^5 3s^2 3p^6 3d^5 4s^2$ to $1s^2 2s^2 2p^4 3s^2 3p^6 3d^5 4s^2$. There can be complex dynamics here and other causes are possible.

XR-HERFD is therefore the perfect tool to investigate these phenomena, as it enables us to observe at exactly what energy shake-off processes occur and their relative magnitude.

Atomic and Solid State Physics Working Together

Some Highlights of this Conference:

- Earlier today: **Hamish Melia, atomic theory and experiment: MCHDF theory and experiment for Cu K$\alpha_{3,4}$**
- **Paul di Paschale [La Trobe: Quantum Interference for X-ray Optics: Phase and Amplitude],**

Posters:

Tuesday: Jonathan Dean [Measuring X-ray spectra of 3d transition metals to World-best accuracy & resolution], Jack Webster [CSIRO: Detectors for Mars], Feng Wang [Quantum Chemistry]

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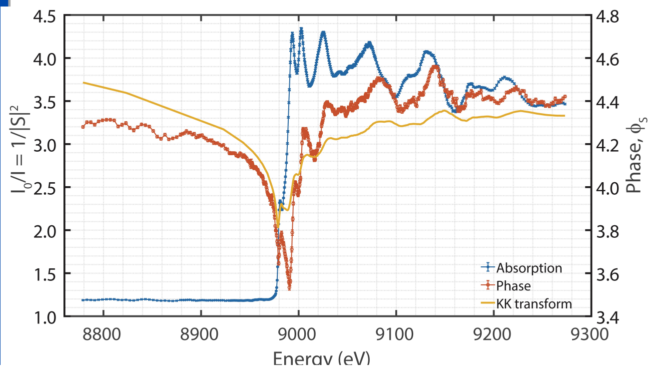

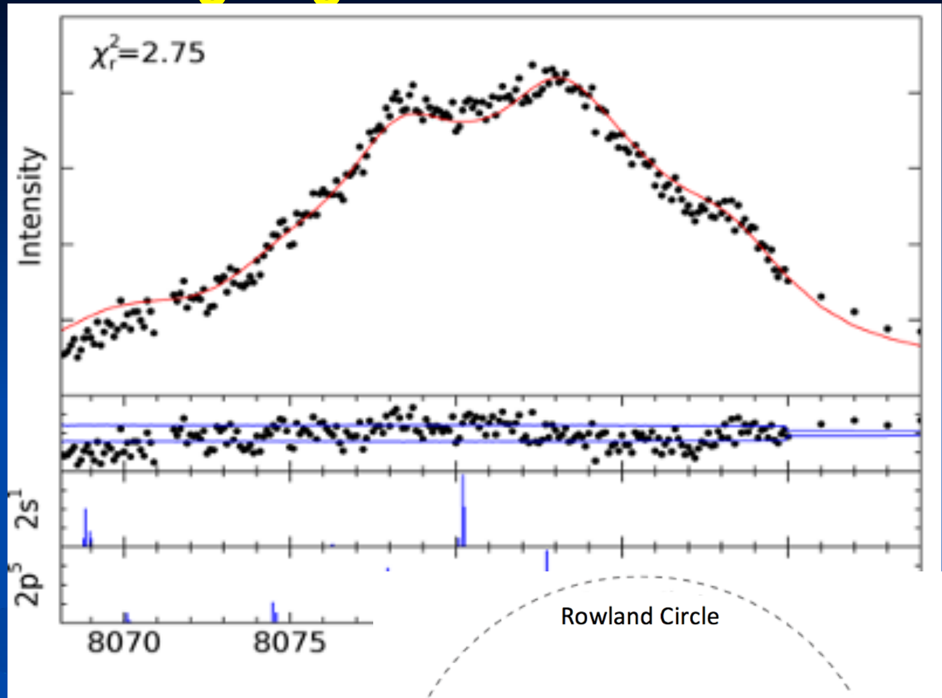

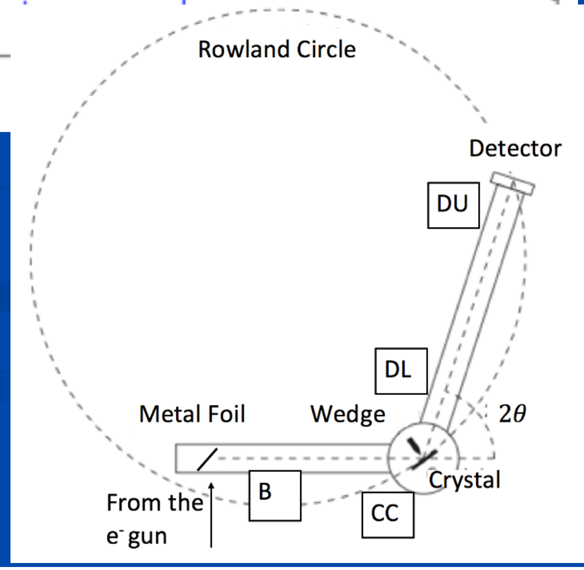

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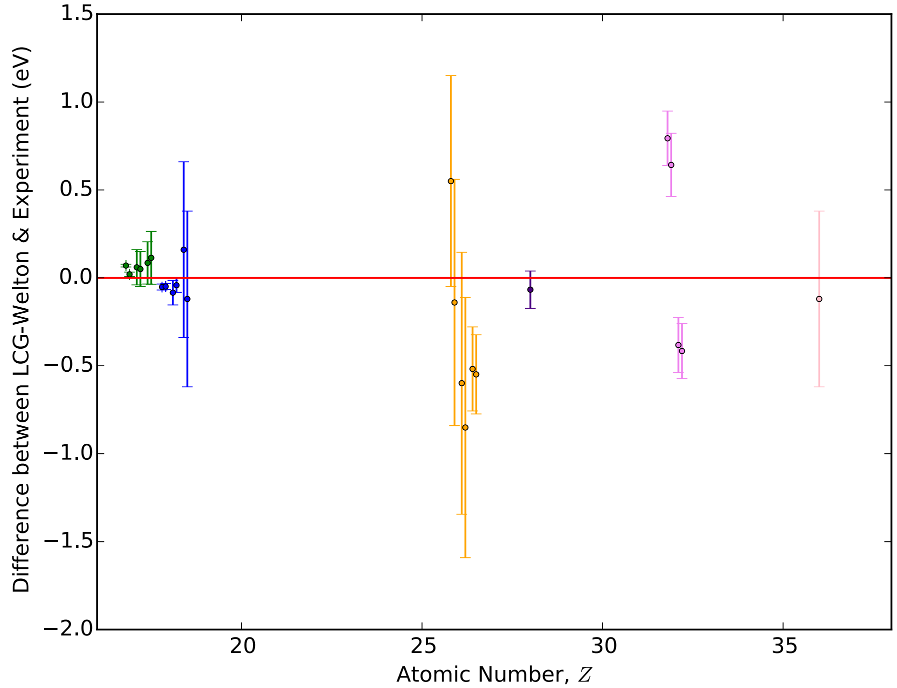

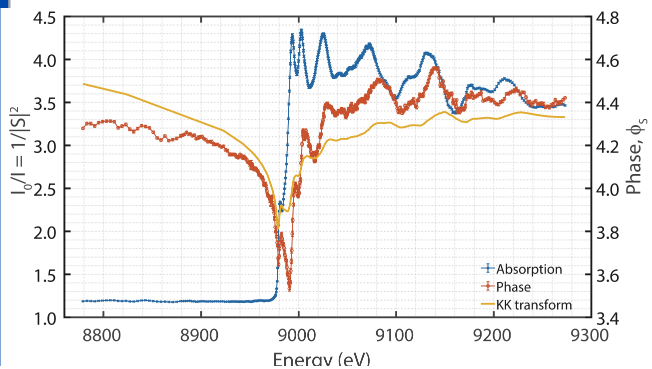

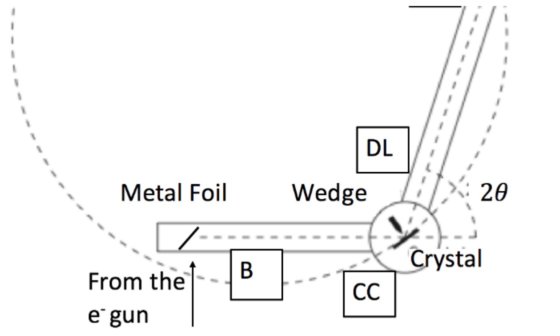

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