X-Ray interactions With Superheavy Atoms

Pavlo Baranov

Queens College

Advisor: John Rehr

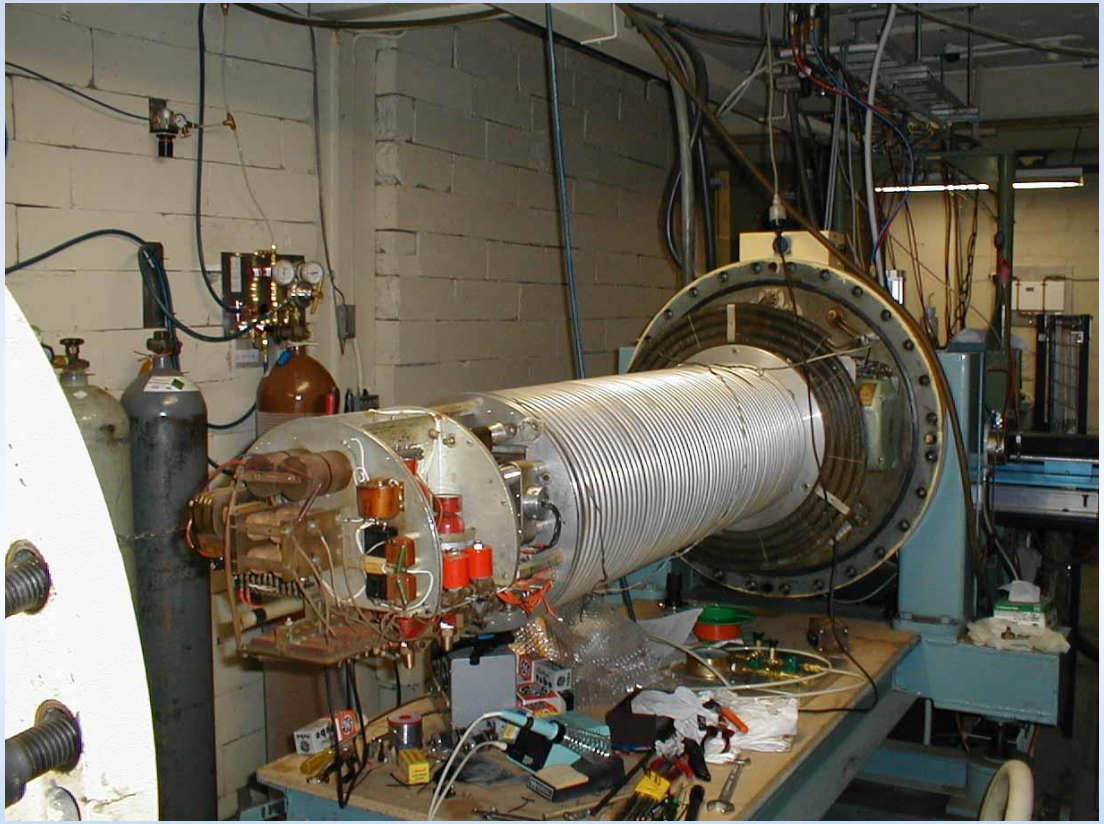
August 18th, 2016

Table of Contents

Introduction

Superheavy Elements

- Start from Z = 104
- Have very short half-lives
- Made artificially
- Created in a particle accelerator



Particle Accelerator, https://upload.wikimedia.org/wikipedia/commons/5/5f/2mv_accelerator-MJC01.jpg

Extended Periodic Table

(Superheavy elements may not exist, and may not follow the order of this table even if they do)

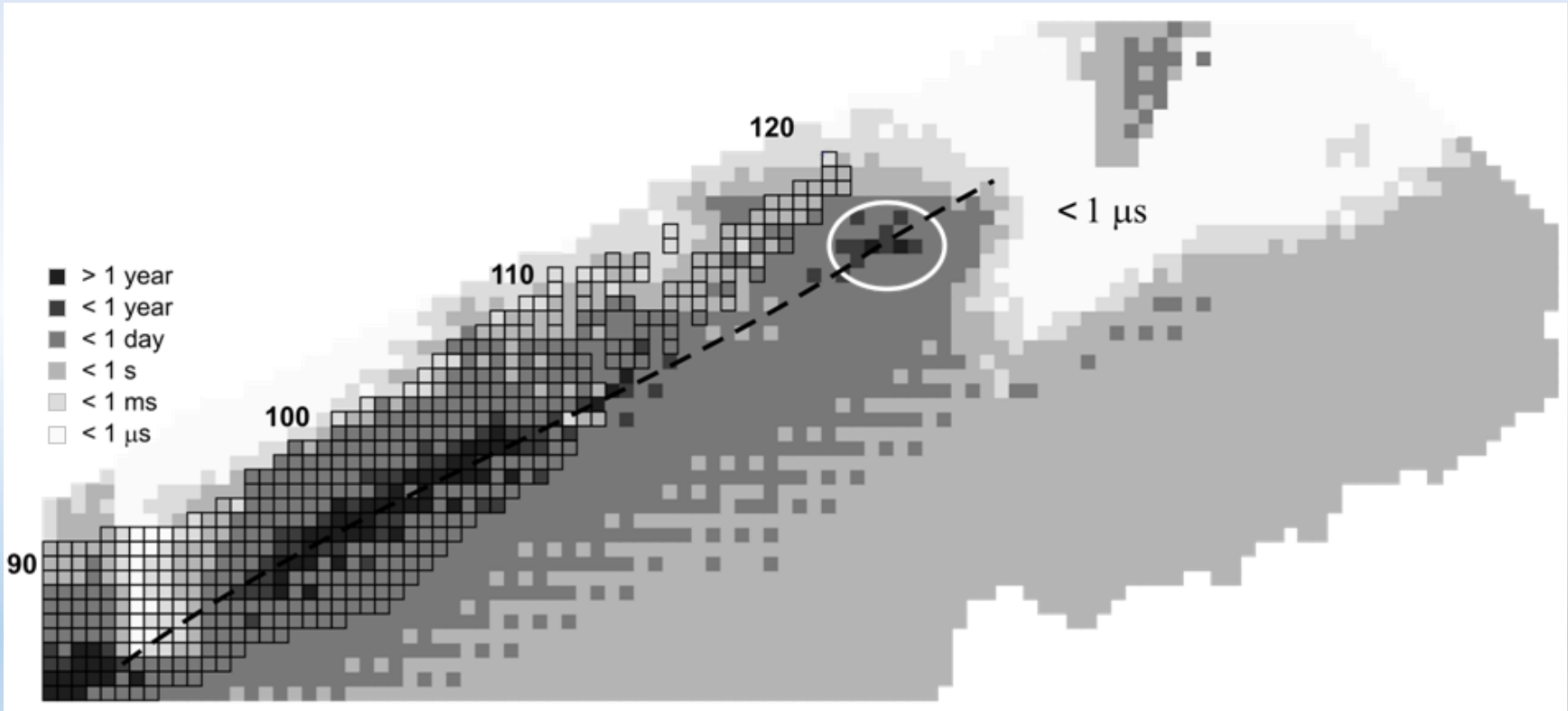
1	1 H																	2 He
2	3 Li	4 Be													5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg													13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo
8	119 Uue	120 Ubn	121 Ubu	122 Ubb	123 Ubt	124 Ubq	125 Ubp	126 Ubh	127 Ubs	128 Ubo	129 Ube	130 Utn	131 Utu	132 Utb	133 Utt	134 Utq	135 Utp	136 Uth	137 Uts	138 Uto	139 Ute	140 Uqn	141 Uqu	142 Uqb	143 Uqt	144 Uqq	145 Uqp	146 Uqh	147 Uqs	148 Uqo	149 Uqe	150 Upn	151 Upu	152 Upb	153 Upt	154 Upq	155 Upp	156 Uph	157 Ups	158 Upo	159 Upe	160 Uhn	161 Uhu	162 Uhb	163 Uht	164 Uhq	165 Uhp	166 Uhh	167 Uhs	168 Uho
9	169 Uhe	170 Usn	171 Usu	172 Usb	173 Ust																																					

Extended Periodic Table, https://sciencepicks.files.wordpress.com/2011/12/extended-periodic-table.png

Why study them???

Island of Stability

- The idea that heavy elements near the isotope ^{300}Ubn (element 120) with near the magic number of protons and neutrons will be much more stable.



Island of Stability, https://upload.wikimedia.org/wikipedia/commons/7/7b/Island_of_Stability_derived_from_Zagrebaev.png

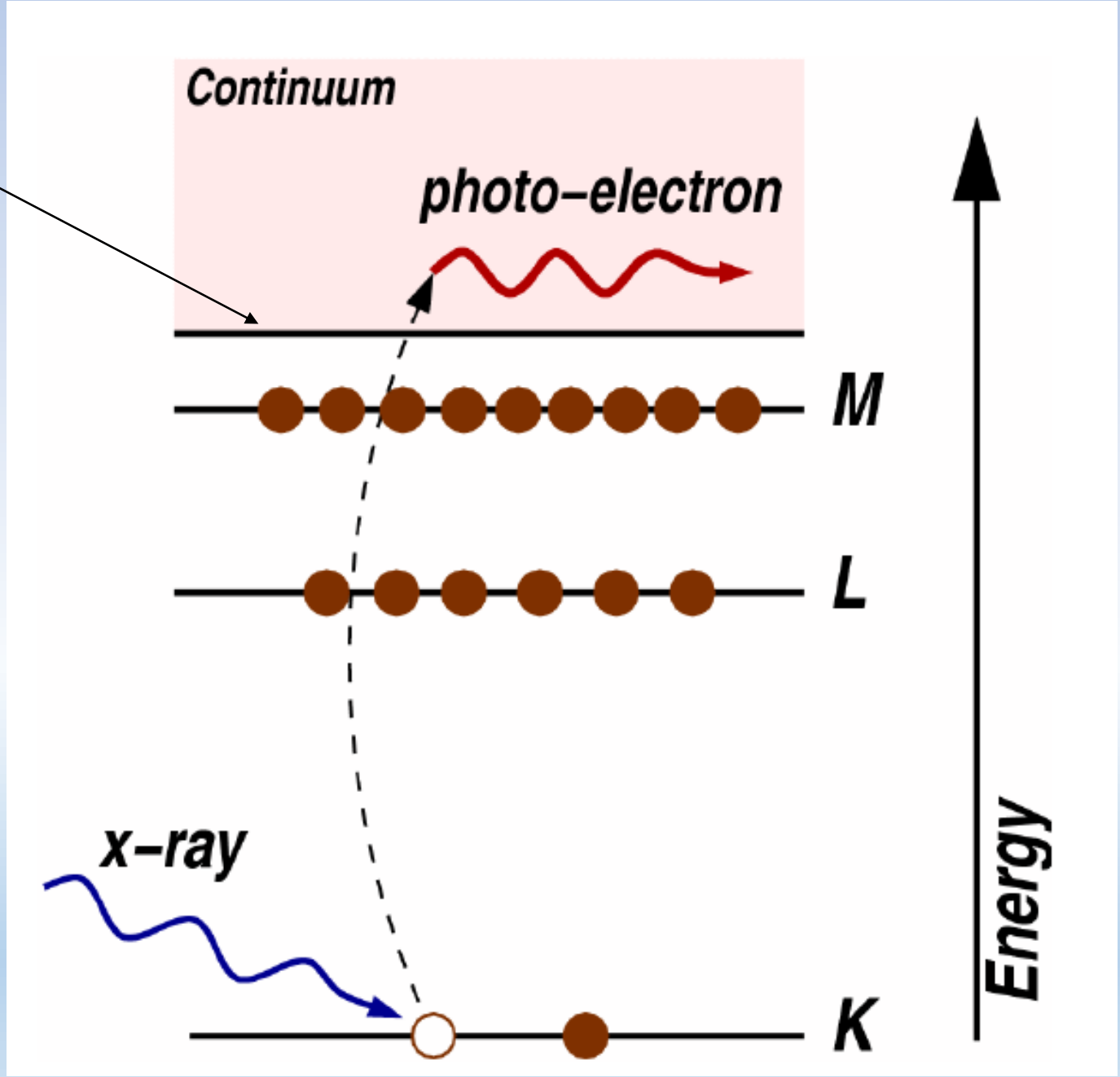
XAFS Theory

XAFS – X-Ray Absorption Fine Structure

- XAFS tells us how x-rays are absorbed by a system of atoms, including free atoms, molecules and solids at energies around the core-level binding energies of the atom.
- XAFS depends on the atomic structure and electronic and vibrational properties of the material; therefore, XAFS can be calculated for every element on the periodic table.
- XAFS can be used to characterize materials, including atomic and electronic structure.
- Absorption coefficient μ, $I = I_0 e^{-\mu t}$ Beer's Law.
- $\mu \propto \sum_f |\langle i|d|f\rangle|^2 \delta(E_f - E_i - \hbar\omega)$ - Fermi's Golden Rule.

Photoelectric Effect

Fermi Level



EXAFS – Extended X-Ray Absorption Fine Structure

- Edges are the sharp rises in absorption at certain energies. They occur at roughly the binding energy of each core-level electron.
- EXAFS is what is happening well above the edges.
- EXAFS Equation

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

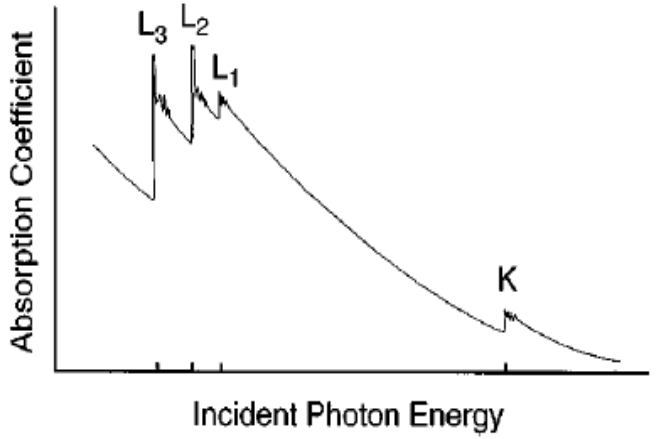
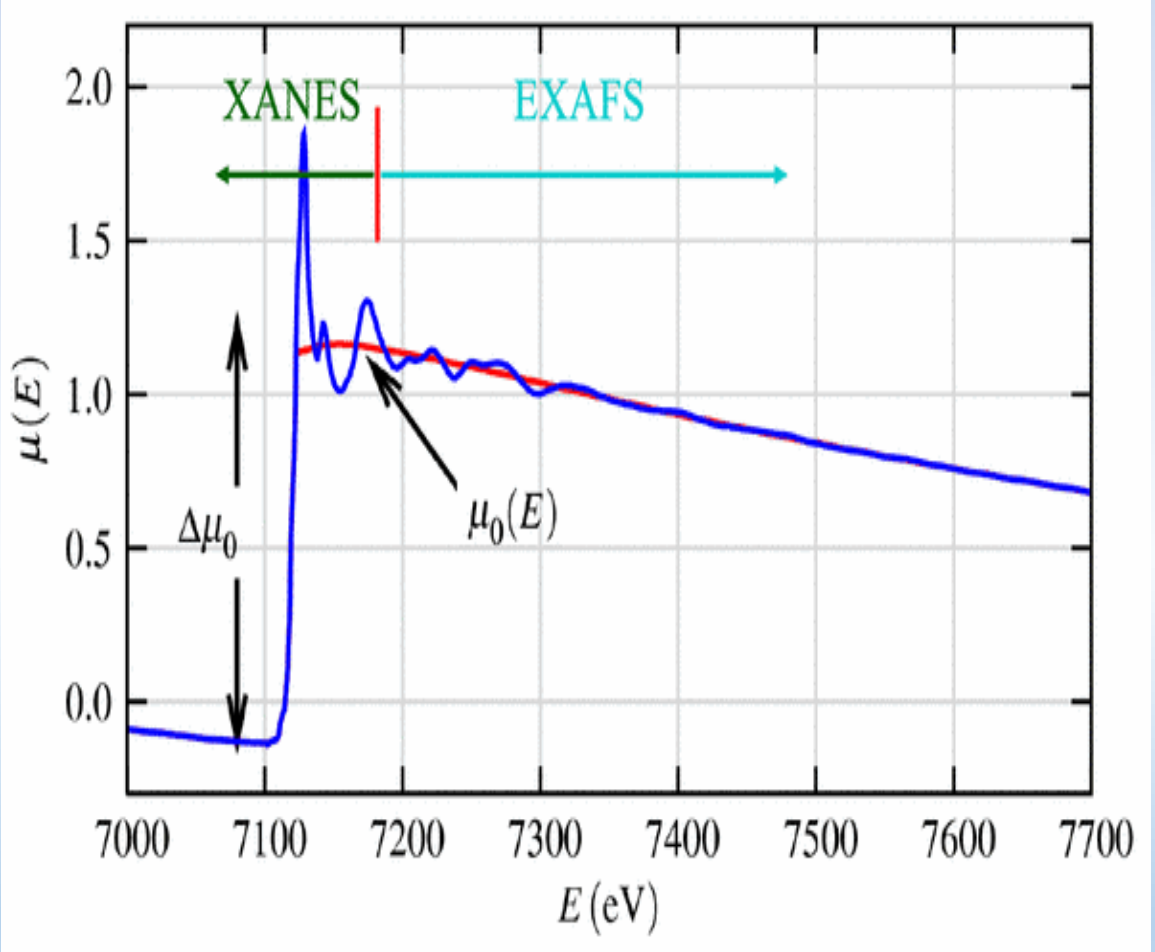


FIG. 2. Schematic view of x-ray absorption coefficient as a function of incident photon energy. Four x-ray edges are shown: K, L_1, L_2, and L_3. Note that the overall decrease in absorption as a function of energy is punctuated by four sharp, step-function-like increases at each edge. Above each edge are the oscillatory wiggles known as the EXAFS. This figure was redrawn; it is based on Fig. I.2 of Müller (1980).

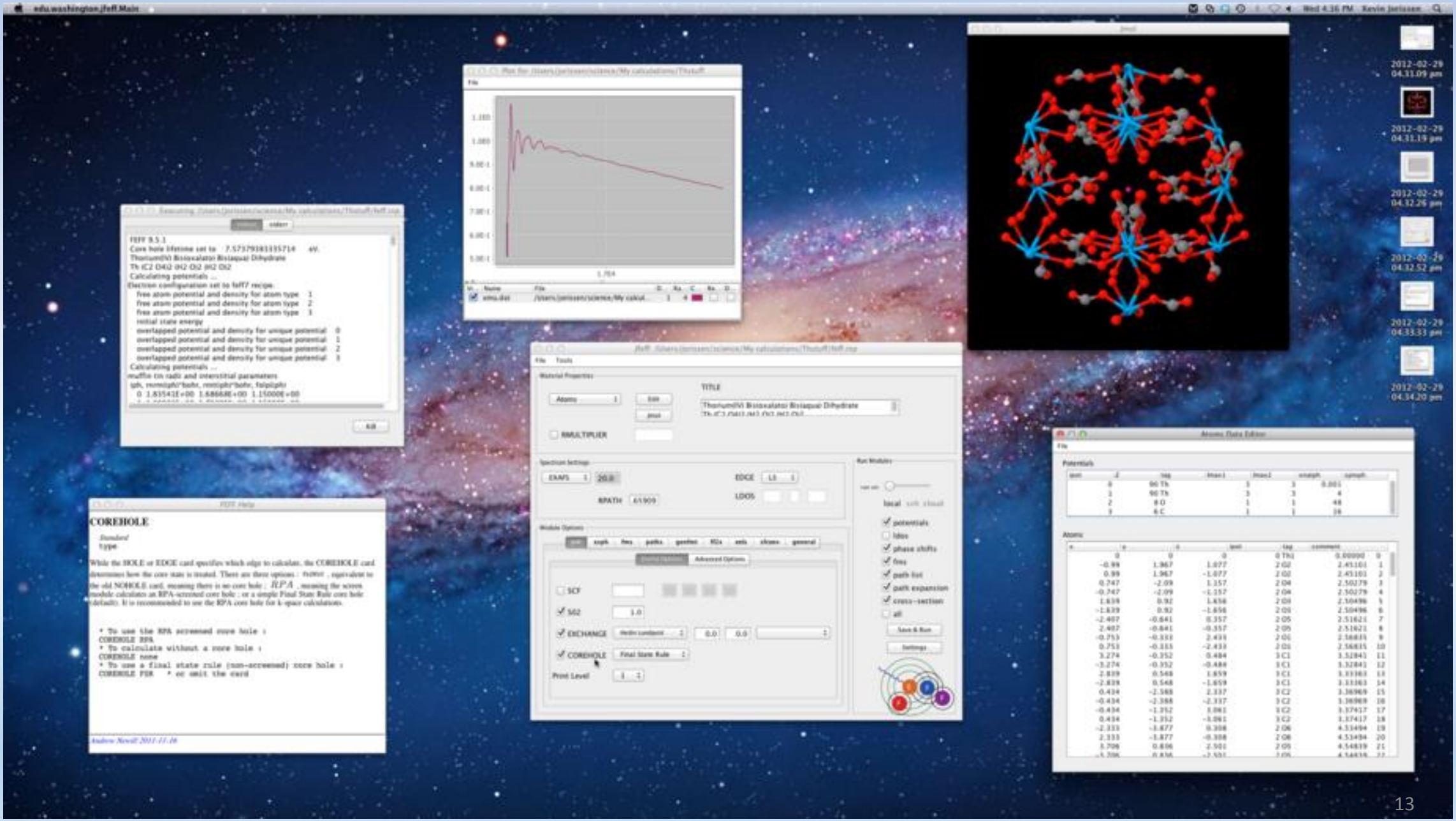
XANES – X-Ray Absorption Near Edge Structure

- XANES is typically within 30 eV of the main absorption edge.
- XANES can be used as a fingerprint to identify the presence of a particular chemical species.

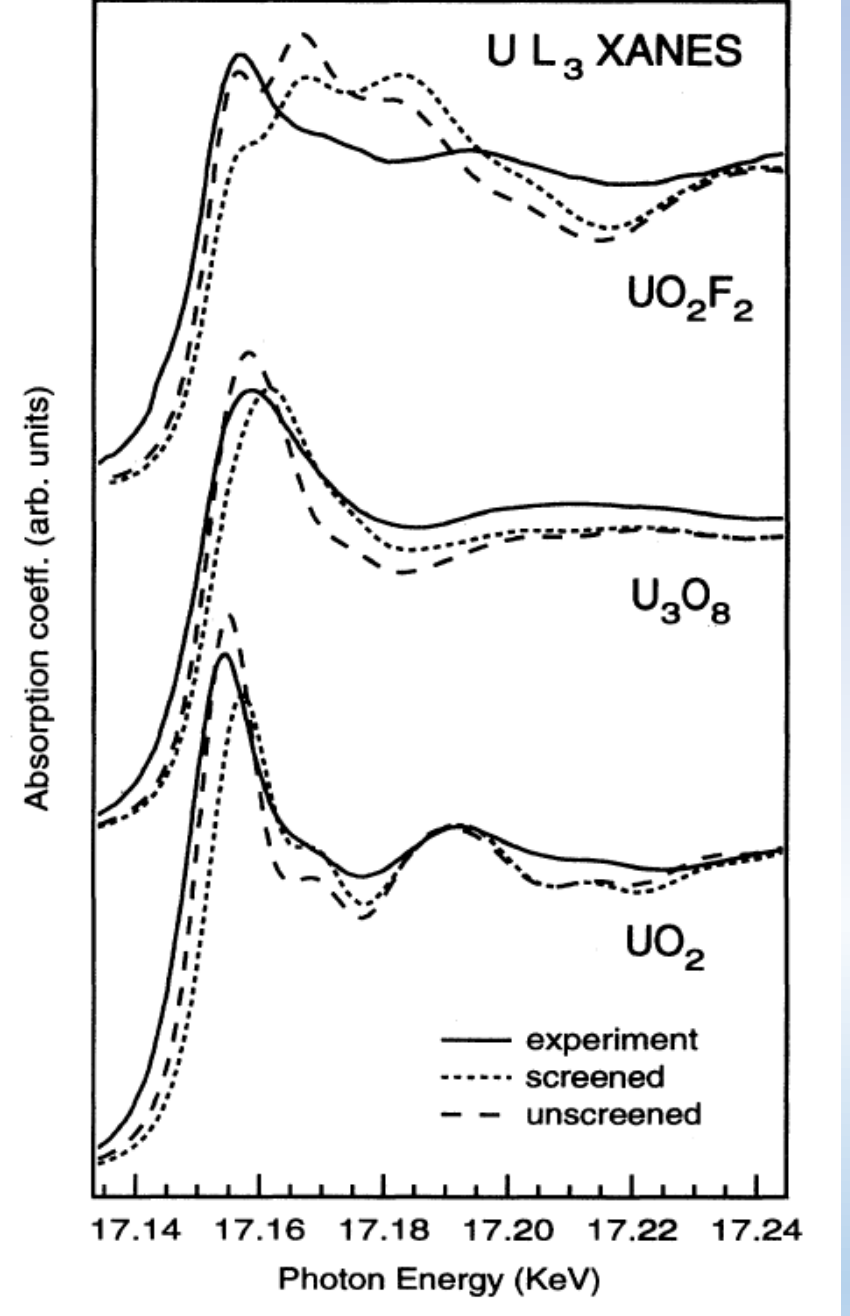


XANES and EXAFS, http://www.ati.ac.at/typo3temp/pics/617d72ef66.png

FEFF9

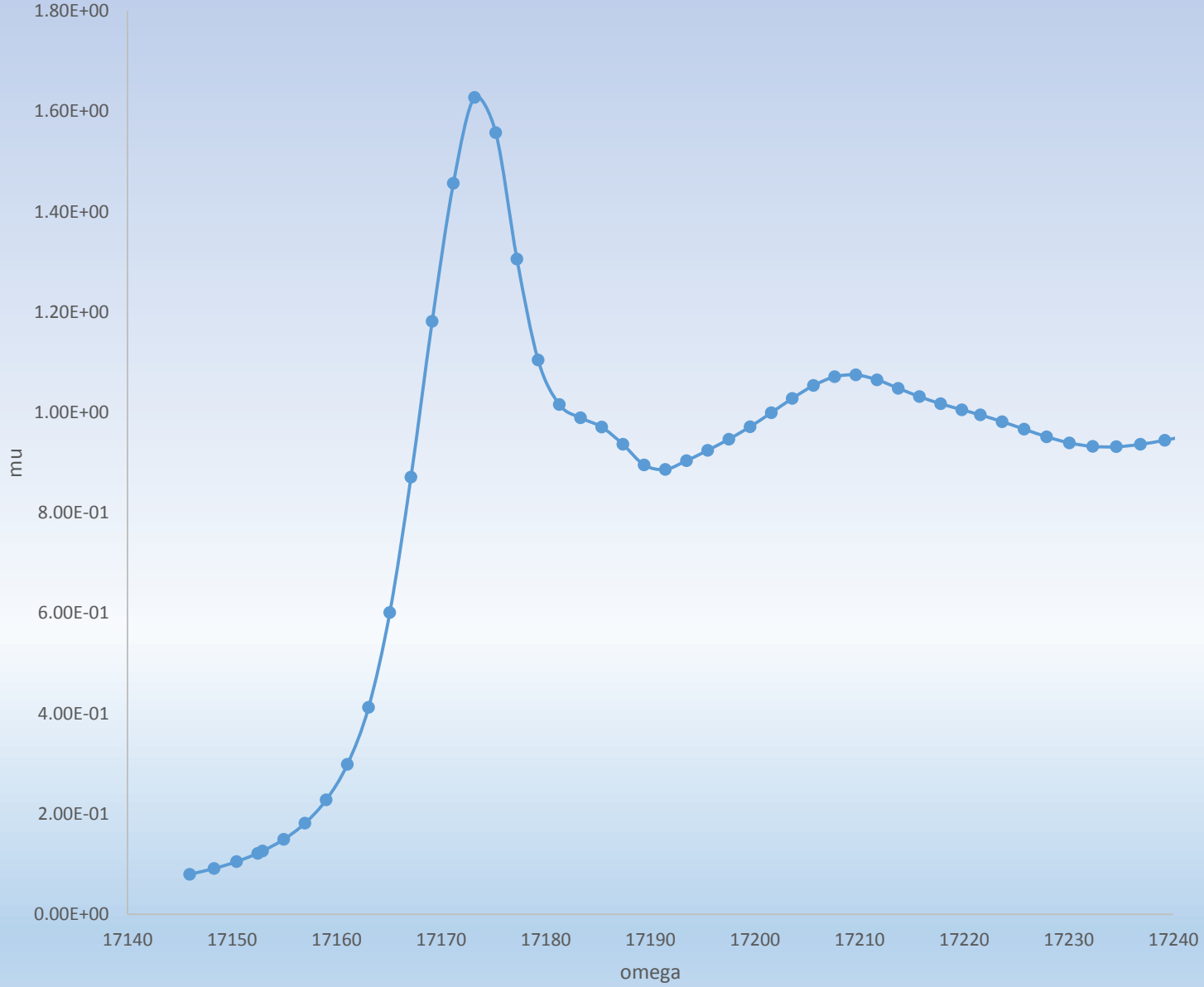


FEFF9, http://www.feffproject.org/feffproject-feff.html



E. A. Hudson, J. J. Rehr, J. J. Bucher, *Multiple-scattering calculations of the uranium L3-edge x-ray-absorption near-edge structure,* Physical Review B, 1995

Uranium Dioxide UO_2



Erbium Oxide Er_2O_3

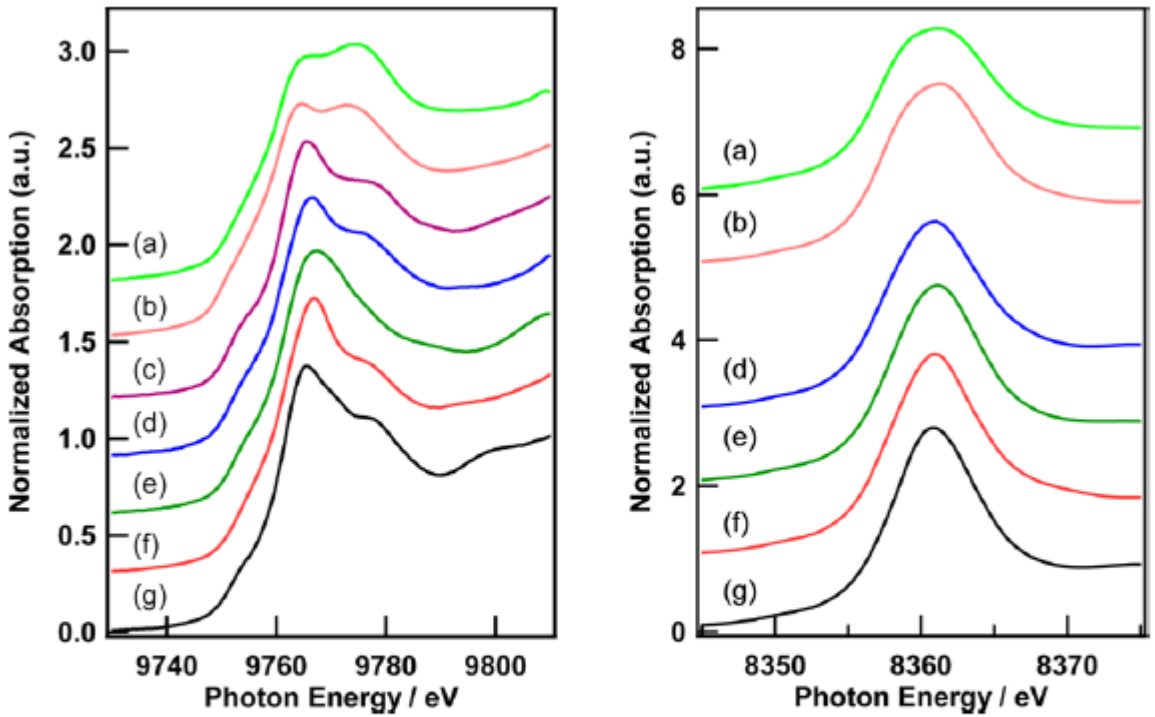
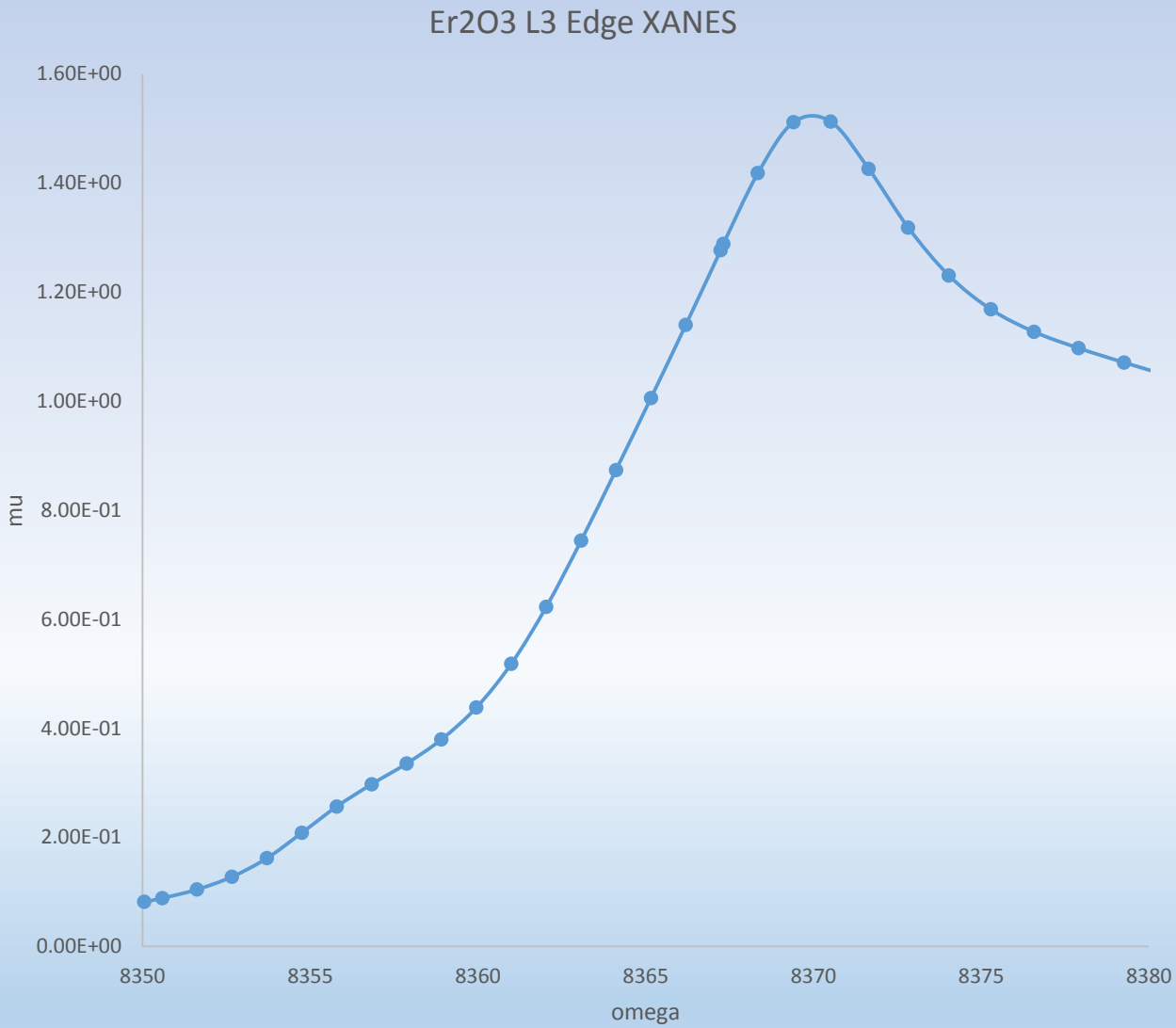
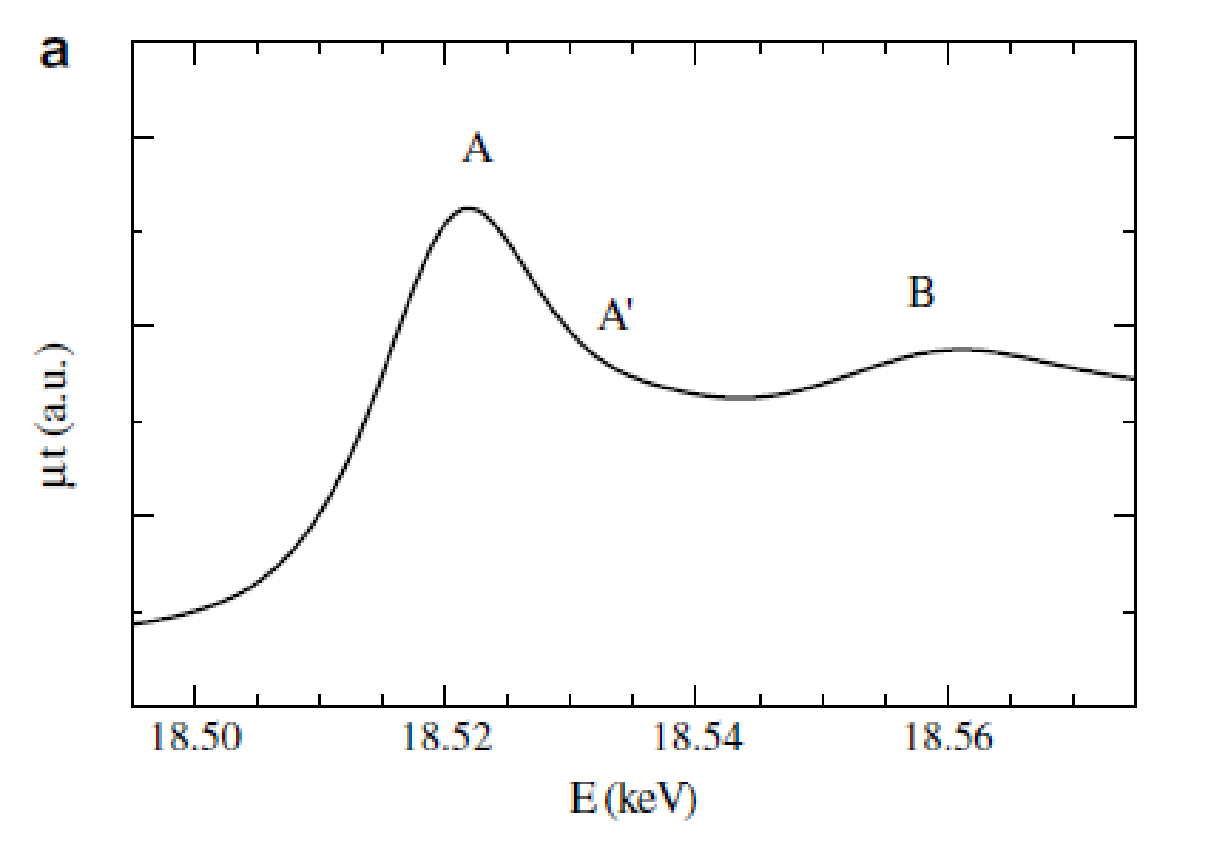


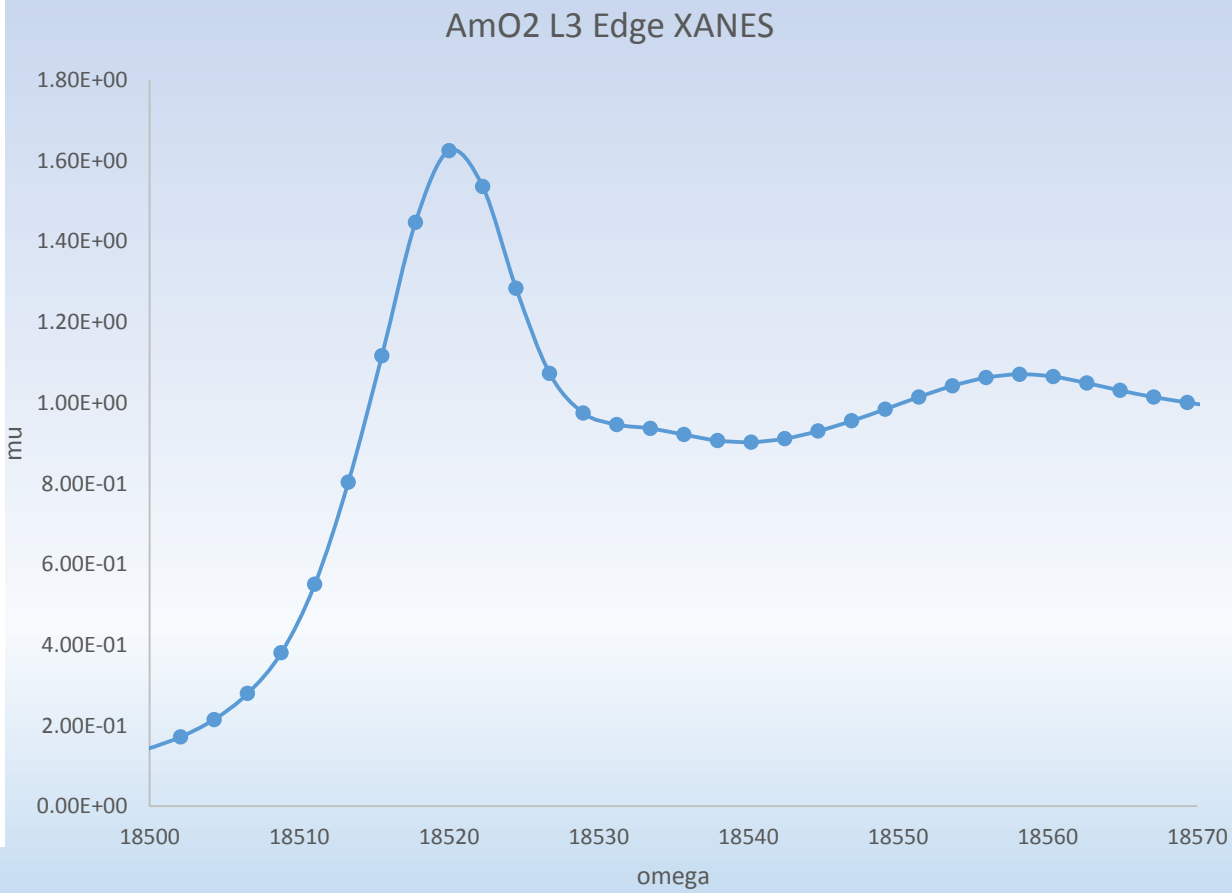
Figure 5. Er L_1- (left) and L_3-edge (right) XANES spectra of Er oxides: (a) $Er_2Cu_2O_5$, (b) Er_2O_3, (c) $BaNiEr_2O_5$, (d) $BaCuEr_2O_5$, (e) $ErNbO_4$, (f) $Er_3Al_5O_{12}$, and (g) $ErVO_4$.

Hiroyuki Asakura, Tetsuya Shishido, Kentaro Teramura, and Tsunehiro Tanaka, *Local Structure and L1- and L3-Edge X-ray Absorption Near Edge Structure of Late Lanthanide Elements (Ho, Er, Yb) in Their Complex Oxides,* J. Phys. Chem. C 2015, 119, 8070−8077



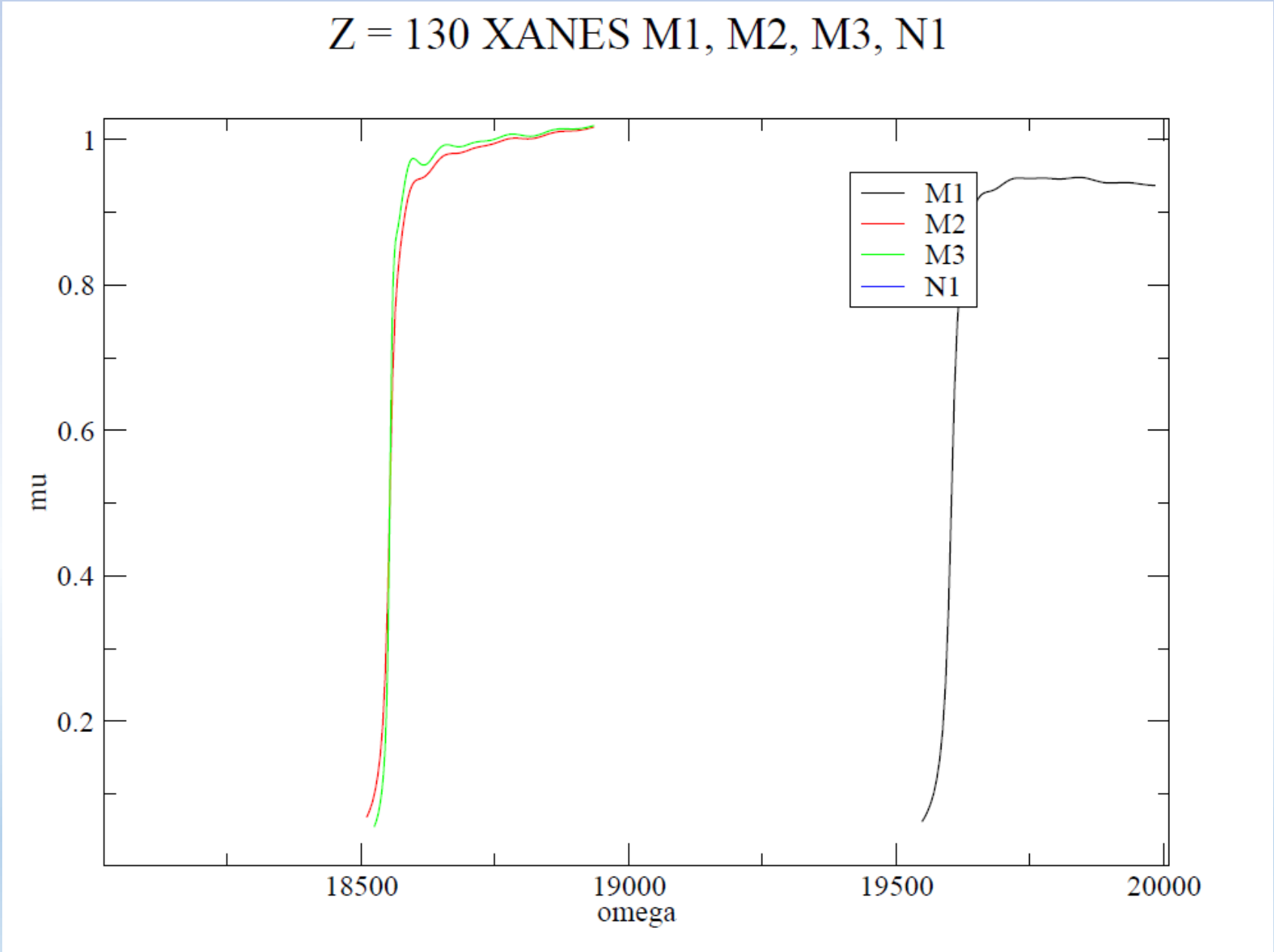
Americium Dioxide AmO_2





Tsuyoshi Nishi, Masami Nakada, Akinori Itoh, Chikashi Suzuki, Masaru Hirata, Mitsuo Akabori, *EXAFS and XANES Studies of Americium Dioxide with fluorite structure,* J. Of Nuclear Materials, 2007

XANES of Untrinilium (Utn2)



Thomson Scattering Cross Section
&
Thomas-Fermi Model

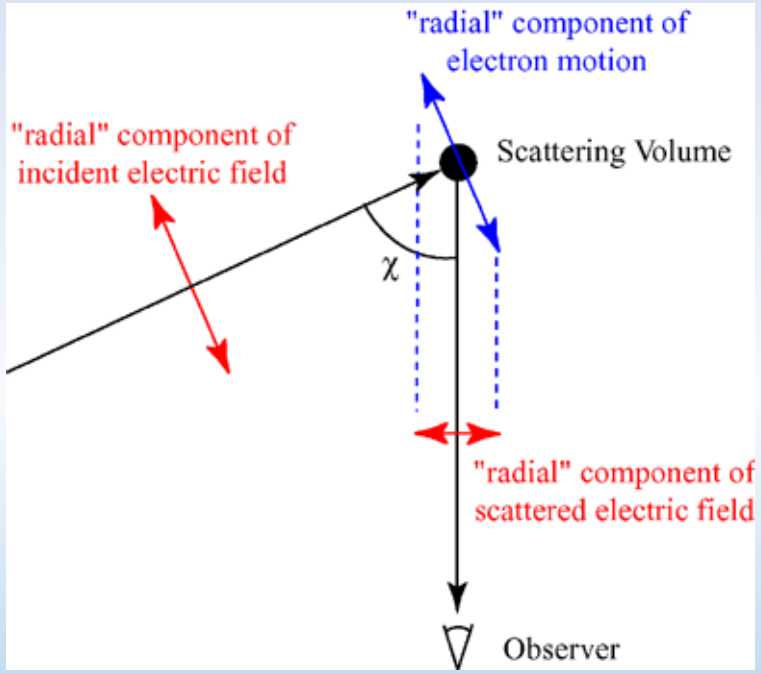
Thomson Scattering

- The elastic scattering of X-rays from free electrons.
- The atomic scattering factor

$$f_0 = \sum_{n=1}^{Z} \int_0^{\infty} 4\pi r^2 \rho_n(r) \frac{\sin(qr)}{qr} dr$$

- Momentum transfer

$$q = \frac{4\pi \sin(\theta_B)}{\lambda}$$

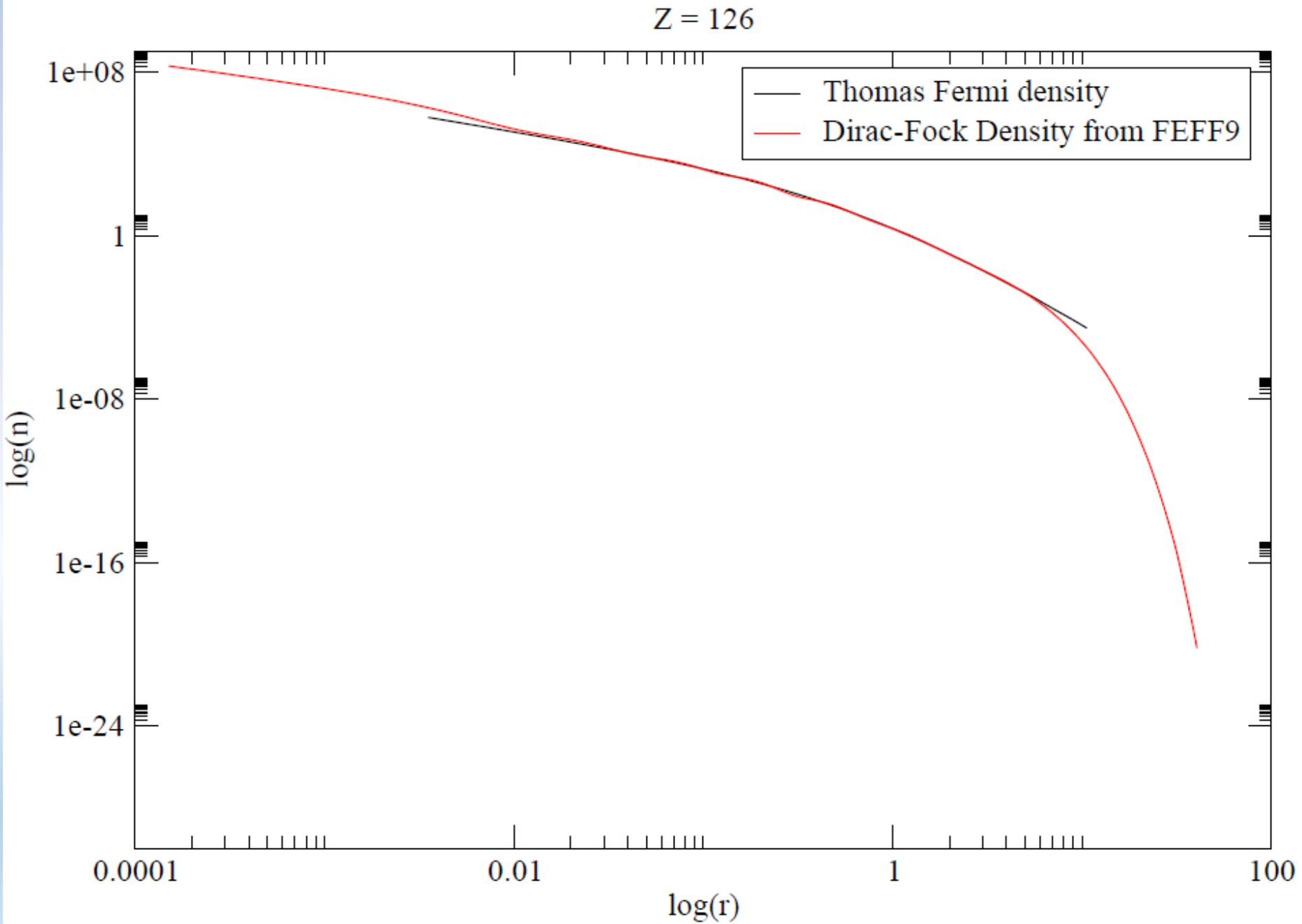


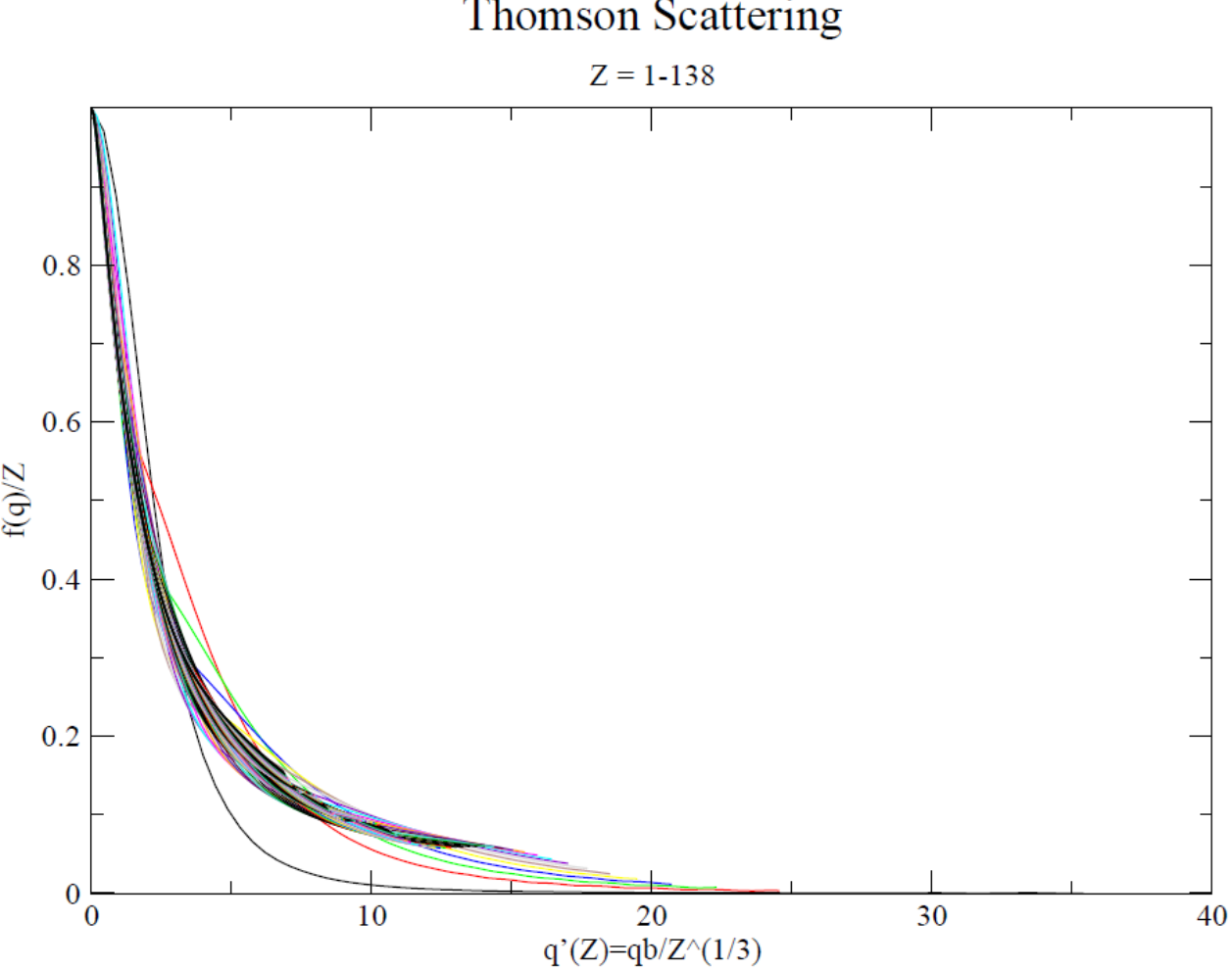
Thomson Scattering, https://upload.wikimedia.org/wikipedia/commons/b/bf/Thomson_scattering_geometry.png

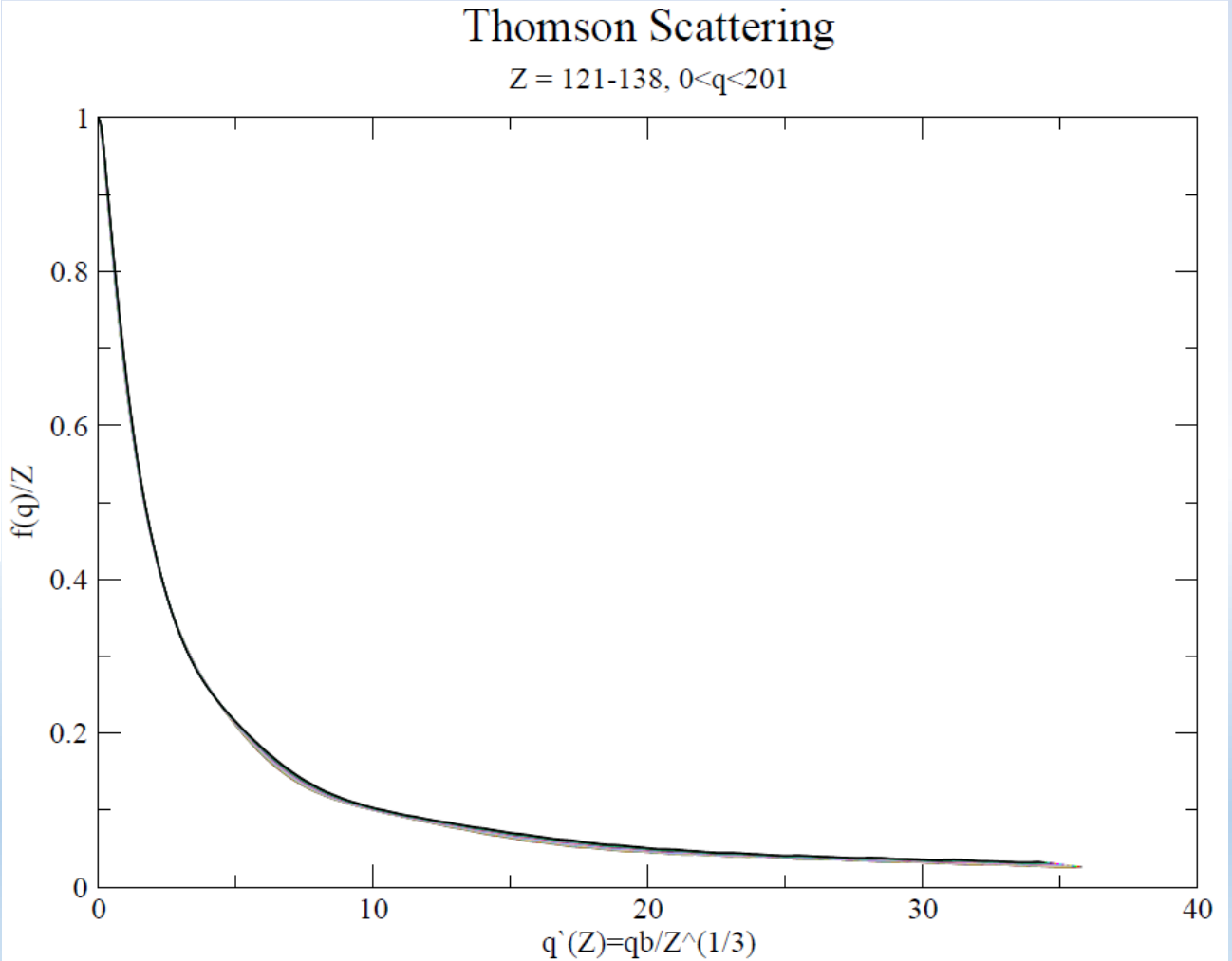
Thomas Fermi model

- $n = \frac{[2(\varphi - \varphi_0)]^{3/2}}{3\pi^2}$
- $r = xbZ^{-1/3}, b = 0.885$
- $\varphi(r) = \frac{Z^{4/3}}{b}\frac{\chi(x)}{x}$
- Thomas Fermi equation $x^{1/2}\frac{d^2\chi}{dx^2} = \chi^{3/2}$
- TF density $n(r) = Z^2 f(\frac{rZ^{1/3}}{b}), f(x) = \frac{32}{9\pi^3}(\frac{\chi}{x})^{3/2}$

Density vs. radius for Thomas Fermi and FEFF9




Thomson Scattering
Z = 1-138
f(q)/Z
q`(Z)=qb/Z^(1/3)
0
0.2
0.4
0.6
0.8
0
10
20
30
40


Thomson Scattering
Z = 121-138, 0<q<201
f(q)/Z
q`(Z)=qb/Z^(1/3)
0
0.2
0.4
0.6
0.8
1
0
10
20
30
40

Future Work

- Calculation of phase shifts using FEFF9
- Comparison to WKB approximation
- Developing a model to calculate radii for superheavy molecules.

Acknowledgments

Thank you to professor John Rehr, Joshua Kas, and Fernando Vila for their guidance through my projects.

Thank you to Ron Musgrave for the machine shop lessons.

Thank you to REU coordinators and the NSF.

References

J. J. Rehr, R. C. Albers, *Theoretical Approaches to X-ray Absorption Fine Structure,* Reviews of Modern Physics, Vol. 72, No. 3, 2000

Pekka Pyykko, *A suggested Periodic Table up to Z ≤ 172, based on Dirac-Fock calculations on atoms and ions,* Phys. Chem. Chem. Phys., 2011,13, 161-168

Hiroyuki Asakura, Tetsuya Shishido, Kentaro Teramura, and Tsunehiro Tanaka, *Local Structure and L1- and L3-Edge X-ray Absorption Near Edge Structure of Late Lanthanide Elements (Ho, Er, Yb) in Their Complex Oxides,* J. Phys. Chem. C 2015, 119, 8070−8077

Tsuyoshi Nishi, Masami Nakada, Akinori Itoh, Chikashi Suzuki, Masaru Hirata, Mitsuo Akabori, *EXAFS and XANES Studies of Americium Dioxide with fluorite structure,* J. Of Nuclear Materials, 2007

E. A. Hudson, J. J. Rehr, J. J. Bucher, *Multiple-scattering calculations of the uranium L3-edge x-ray-absorption near-edge structure,* Physical Review B, 1995

Matthew Newville, *Fundamentals of XAFS,* Consortium for Advanced Radiation Sources, 2004

J. Kas, *Theory and Calculation of X-Ray Absorption,* https://www.bnl.gov/ps/nsls/workshops/2006/exafs/talks/Kas.pdf, 2006

V. L. Eletskii, V.S. Popov, *The Thomas-Fermi method for Z>137,* Zh. Eksp. Teor. Fiz. 73, 2046-2059, 1977

A. Messiah, *Quantum Mechanics,* Dover Publications Inc., Mineola, New York, 1999

L. D. Landau, E. M. Lifshitz, *Quantum Mechanics, non-relativistic theory,* Pergamon Press, Oxford, New York, Beijing, Frankfurt, Sao Paulo, Sydney, Tokyo, Toronto, 1977

Gwyndaf Evans, *Classical X-ray scattering*, http://www.gwyndafevans.co.uk/thesis-html/node11.html, 1994

Ray Wong, Josh Alamillo**,** *EXAFS: Theory,* http://chem.libretexts.org/Core/Physical_Chemistry/Spectroscopy/X-ray_Spectroscopy/EXAFS%3A_Theory, 2016