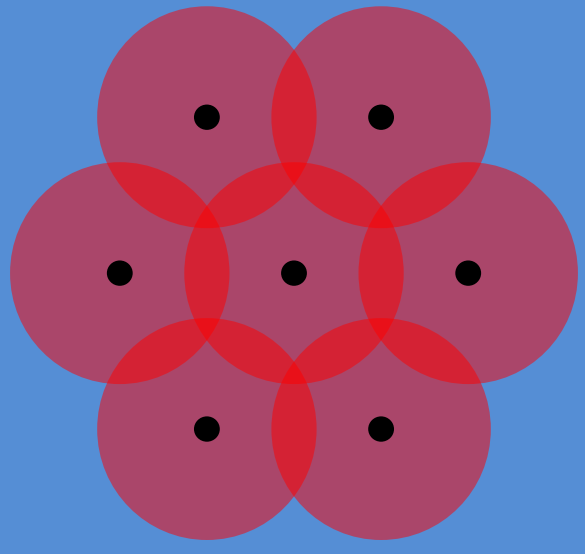
II. Real-space multiple-scattering theory of EXAFS and XANES & FEFF

J. J. Rehr, J. J. Kas and F. D. Vila



UNIVERSITY OF WASHINGTON

TIMES

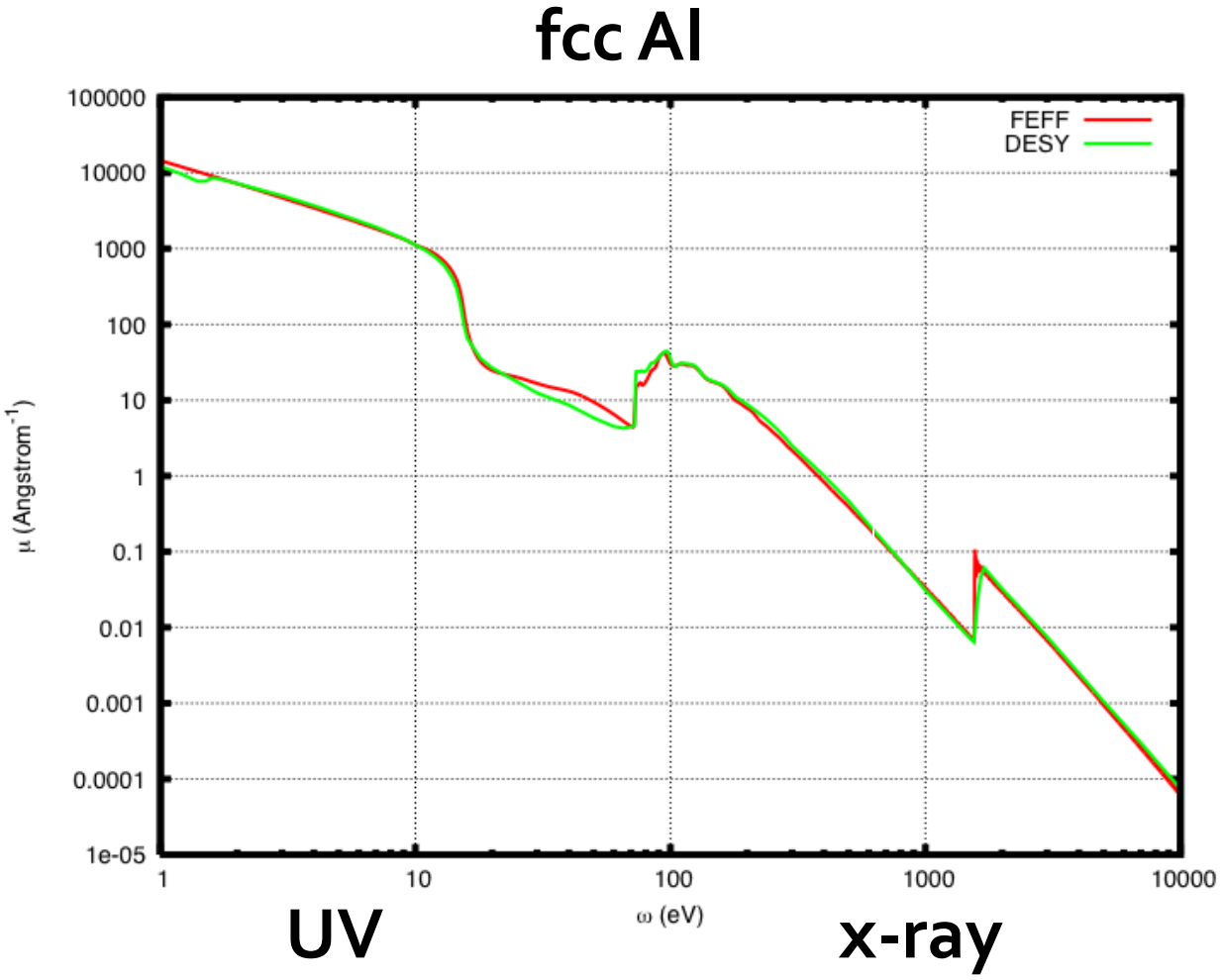
Outline

Talk:

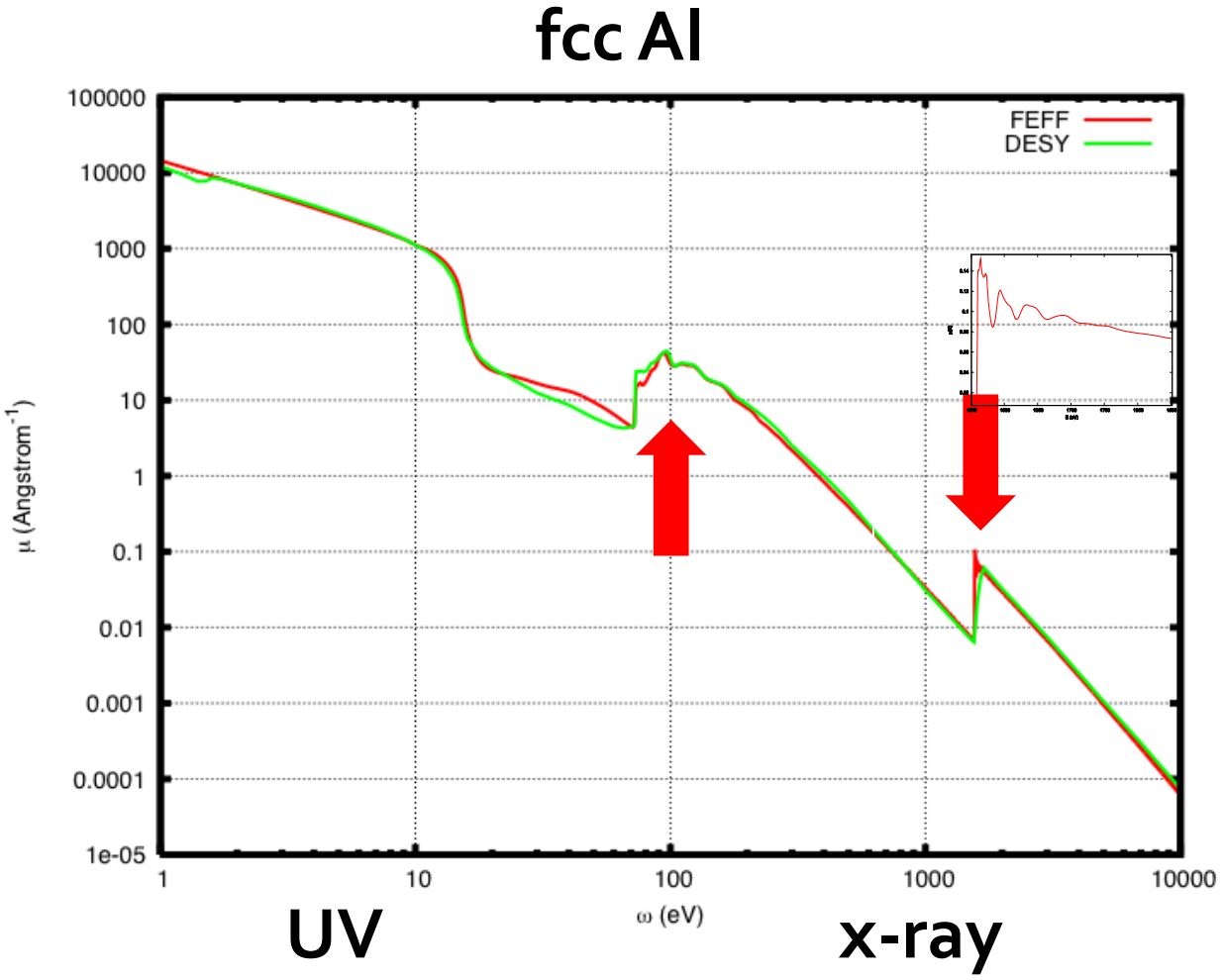
-Real-space multiple-scattering (RSMS) Theory
aka Real-space Green's function (RSGF) theory
-Implementation of RSMS in FEFF

Key approximations and limitations
Effects of structure and disorder
Some advanced developments

Full spectrum XAS: Expt. Vs Theory



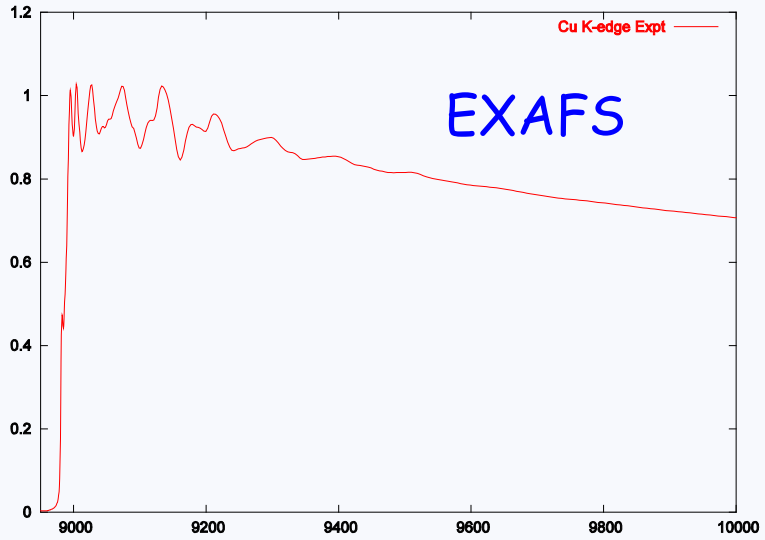
The devil is in the details: edges, fine-structure …

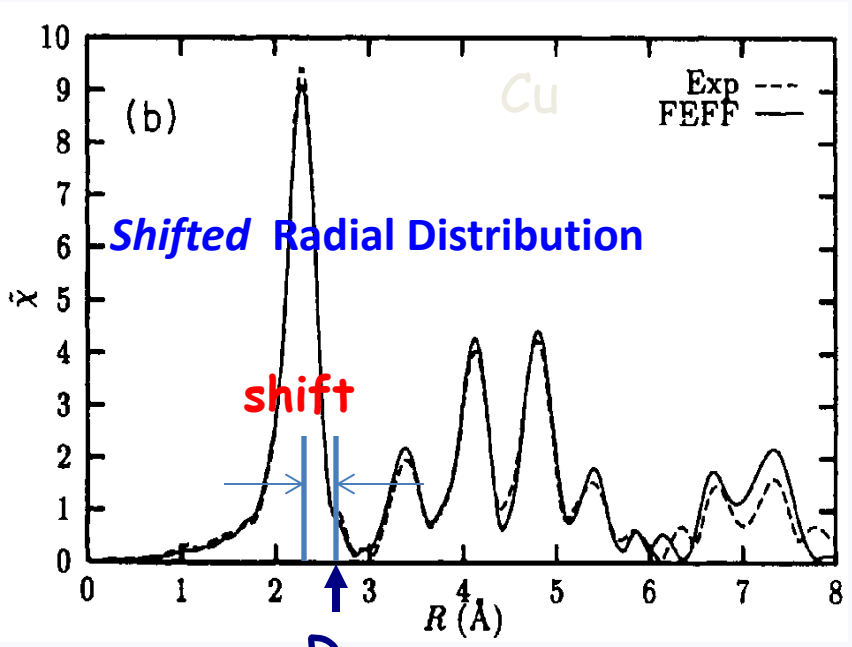


Historical interpretation of EXAFS*

*Stern Sayers Lytle, UW **1971**

Short range order theory → **EXAFS Fourier Transform**



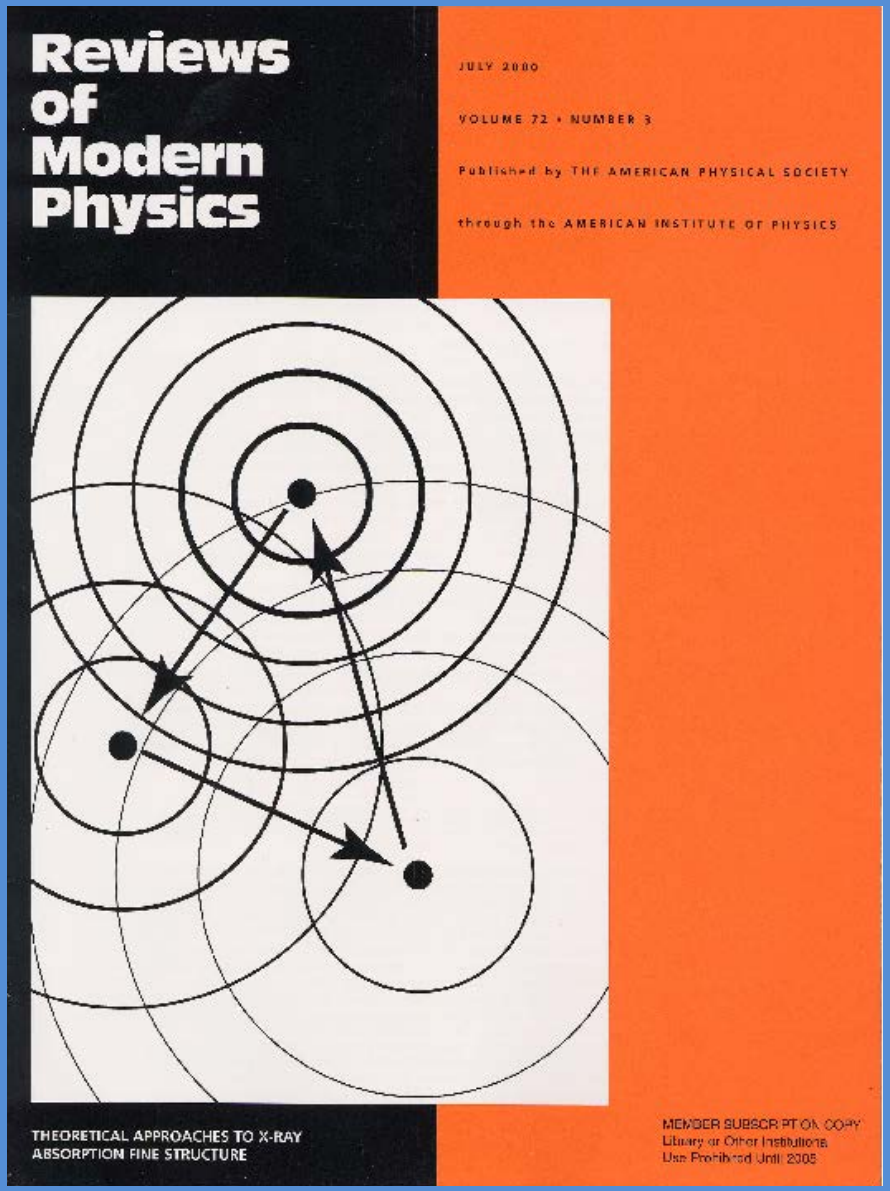


→ X-ray Microscope!

R_{nn}

BUT needed to calibrate experiment with "Standard"

EXAFS Theory

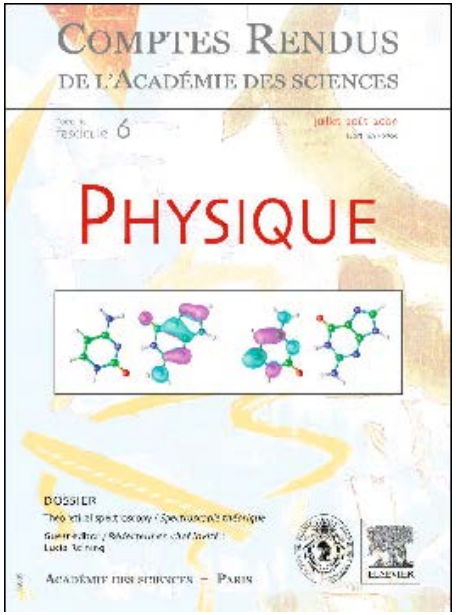


Quantitative theory of EXAFS:

Theory behind FEFF6

J. J. Rehr & R.C. Albers
Rev. Mod. Phys. 72, 621 (2000)

Advances in Theory – FEFF9



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C. R. Physique 10 (2009) 548–559

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Theoretical spectroscopy / Spectroscopie théorique

Ab initio theory and calculations of X-ray spectra

John J. Rehr *, Joshua J. Kas, Micah P. Prange, Adam P. Sorini, Yoshinari Takimoto, Fernando Vila

Department of Physics, University of Washington, Seattle, WA 98195-1560, USA

Available online 5 December 2008

Update of Rehr & Albers: Advanced techniques and ab initio treatment of many-body effects

Other references:

PHYSICAL REVIEW B VOLUME 58, NUMBER 12 15 SEPTEMBER 1998-II

Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure

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(Received 26 September 1997; revised manuscript received 14 April 1998)

PERSPECTIVE www.rsc.org/pccp | Physical Chemistry Chemical Physics

Parameter-free calculations of X-ray spectra with FEFF9

John J. Rehr,*[a] Joshua J. Kas,[a] Fernando D. Vila,[a] Micah P. Prange[bc] and Kevin Jorissen[a]

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DOI: 10.1039/b926434e

RSGF in the hierarchy of spectroscopy methods

sophistication

Atomic models:

e.g. de Groot. Atomic cross-sections, multiplet s
theory with fitted parameters, crystal field model Hamiltonians

DFT (Density Functional Theory):

WIEN2k, ABINIT, VASP, CASTEP , StoBe, Orca …,
Accurate for ground-state properties, not reliable for excited states,
Delta-SCF "Final State Rule" with core-hole

Quasi-particle Green's Function Theory: FEFF9

Appropriate for excited states, NOT full potential

BSE (Bethe-Salpeter Equation):

Exc!ting, OCEAN, AI2NBSE. Accurate but demanding.
Less user friendly. Misses excitations & satellites

QC methods:

MRCI, MRCC, CASPT2, QMC, etc, highly accurate but
mostly intractable except in small molecules

FEFF development philosophy

"Pretty good" spectra

Advantages:

- Real-space
- Fully relativistic, all-electron
- Semi-automated, user-friendly, easy to use
- Built for EXAFS and related x-ray spectroscopies
- Applicable to materials throughout the periodic table

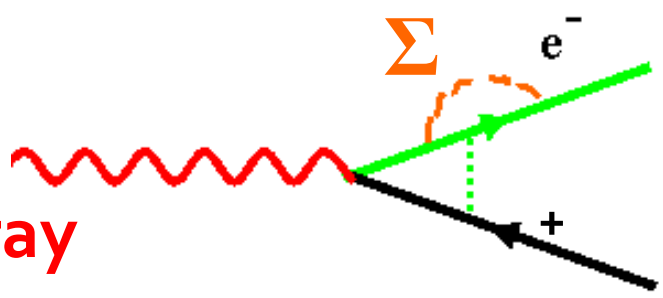
Disadvantages: Not always the best tool:

- Spherical potentials – can lose accuracy near edges
- Quasi-particle theory only – ignores multiplets, satellites

FEFF quantitative XANES theory in one Feynman diagram

Inelastic Losses
Self-energy

Real-Space
Green's Function



Screened
core-hole

"Can you write an equation

for the theory?"

P.A.M. Dirac

Answer: Exact EXAFS Equation*

Effective Scattering Amplitude f_{eff}

$$\chi(k) = S_0^2 \sum_R \frac{|f_{\text{eff}}(k)|}{kR^2} \sin(2kR+\Phi_k) e^{-2R/\lambda_k} e^{-2\sigma^2 k^2}$$

S_0^2 Many body amplitude factor

λ_k Mean free path

σ^2 Mean square vib amplitude

EXAFS measures **local structure & disorder**

Distance R Coordination N Disorder σ^2

*JJR, RC Albers, CR Natoli, EA Stern, Phys Rev B**34**, 4350 (1986)

BUT: need many parameters !

Question: Can the EXAFS parameters

$$k \quad f_{\mathrm{eff}} \quad \Phi_k \quad \sigma^2 \quad \lambda_k \quad S_0^2$$

be calculated theoretically **?**

FEFF: Many-body → effective single particle

XAS absorption coefficient

Many-body Fermi's Golden Rule

$$\mu(\omega) \propto \sum_F |\langle I|\Delta|F\rangle|^2 \, \delta\left(E_F - E_I - \omega\right)$$

Effective Single particle Fermi's Golden Rule

$$\mu(\omega) \propto \sum_{i,f} |\langle i|d|f\rangle|^2 \, \delta\left(E_f - E_i - \omega\right) S_0^2$$

$$H = -(1/2)\nabla^2 + V$$

$$H' = H + V_{ch} + \Sigma(E)$$

FEFF: From sum-over-states to Green's function

Effective Single particle Fermi's Golden Rule

$$\mu(\omega) \propto \sum_{ij} \langle i | d^{\dagger} | f \rangle \langle f | d | i \rangle \, \delta(E_f - E_i - \omega) \; S_0^2$$

FEFF: From sum-over-states to Green's function

Effective Single particle Fermi's Golden Rule

$$\mu(\omega) \propto \sum_{ij} \langle i | d^{\dagger} | f \rangle \langle f | d | i \rangle \, \delta(E_f - E_i - \omega) \quad S_0^2$$

$$\rho(r, r', E) = \sum_f |f\rangle\langle f| \; \delta\left(E_f - E\right)$$

Density Matrix

FEFF: From sum-over-states to Green's function

Effective Single particle Fermi's Golden Rule

$$\mu(\omega) \propto \sum_{ij} \langle i | d^{\dagger} | f \rangle \langle f | d | i \rangle \, \delta(E_f - E_i - \omega) \; S_0^2$$

$$\rho(r, r', E) = \sum_f |f\rangle\langle f| \; \delta\left(E_f - E\right)$$

$$\mathrm{Im}\left[G(r, r', E)\right] = -\frac{1}{\pi}\rho(r, r', E)$$

$$G = \left[E - H + i\Gamma\right]^{-1}$$

Density matrix from Green's function

FEFF: From sum-over-states to Green's function

Effective Single particle Fermi's Golden Rule

$$\mu(\omega) \propto \sum_{ij} \langle i | d^{\dagger} | f \rangle \langle f | d | i \rangle \, \delta(E_f - E_i - \omega) \; S_0^2$$

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$$\mathrm{Im}\left[G(r, r', E)\right] = -\frac{1}{\pi}\rho(r, r', E)$$

$$G = \left[E - H + i\Gamma\right]^{-1}$$

Substitute sum over final states with Green's function

$$\mu(\omega) \propto \mathrm{Im} \sum_i \langle i | d^{\dagger} G(\omega + E_i) d | i \rangle \, \theta_{\Gamma}(\omega + E_i - E_{Fermi}) S_0^2$$

What's a Green's function?

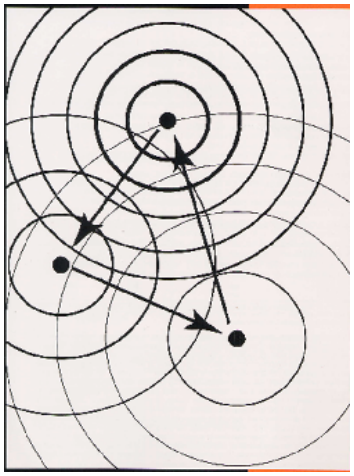
Wave function in QM $H\,\Psi = E\,\Psi$

$\Psi(r)$ = Amplitude to find particle at r

Green's function $(H - E)\,G = -\,\delta(r-r')$

$G(r,r',E)$ = *aka Propagator*

= Amplitude to go from r to r'



FEFF: Local basis and matrix elements

$$\mu(\omega) \propto \mathrm{Im} \sum_i \left\langle i \left| d^\dagger G(\omega + E_i) d \right| i \right\rangle \theta_\Gamma(\omega + E_i - E_{Fermi}) \quad S_0^2$$

Insert complete set of states $1 = \sum_L |i, L\rangle\langle i, L|$

FEFF: Local basis and matrix elements

$$\mu(\omega) \propto \mathrm{Im} \sum_i \langle i | d^\dagger G(\omega + E_i) d | i \rangle \, \theta_\Gamma(\omega + E_i - E_{Fermi}) \; S_0^2$$

Insert complete set of states $1 = \sum_L |i, L\rangle\langle i, L|$

$$\mu(\omega) \propto \mathrm{Im} \sum_{iLL'} \langle i | d^\dagger | i, L \rangle \, G_{LL'}(\omega + E_i) \, \langle i, L' | d | i \rangle \, \theta_\Gamma(\omega + E_i + E_{Fermi}) \; S_0^2$$

FEFF: Local basis and matrix elements

$$\mu(\omega) \propto \mathrm{Im} \sum_i \langle i | d^\dagger G(\omega + E_i) d | i \rangle \, \theta_\Gamma(\omega + E_i - E_{Fermi}) \; S_0^2$$

Insert complete set of states $1 = \sum_L |i, L\rangle\langle i, L|$

Matrix elements

$$\mu(\omega) \propto \mathrm{Im} \sum_{iLL'} \langle i | d^\dagger | i, L \rangle \, G_{LL'}(\omega + E_i) \, \langle i, L' | d | i \rangle \, \theta_\Gamma(\omega + E_i + E_{Fermi}) \, S_0^2$$

Green's Function matrix

Getting *G*: Multiple Scattering Theory

Dyson's equation: $G = G^0 + G^0 V G$

Iterating: $G = G^0 + G^0 V G^0 + G^0 V G^0 V G^0 + \cdots$

Getting *G*: Multiple Scattering

Dyson's equation: $G = G^0 + G^0 V G$

Iterating: $G = G^0 + G^0 V G^0 + G^0 V G^0 V G^0 + \cdots$

$$G(r,r') = G_0(r,r') + \int d^3 r'' G_0(r,r'') V(r'') G_0(r'',r') + \cdots$$

Getting *G*: Multiple Scattering

Dyson's equation: $G = G^0 + G^0 V G$

Iterating: $G = G^0 + G^0 V G^0 + G^0 V G^0 V G^0 + \cdots$

Atomic pot. partition $V = \sum_i v_i$

$$G = G^0 + \sum_i G^0 v_i G^0 + \sum_{ij} G^0 v_i G^0 v_j G^0 + \ldots$$

Getting *G*: Multiple Scattering

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Site scatt. matrix $t_i = v_i + v_i G_0 t_i$ $G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$

Getting *G*: Multiple Scattering

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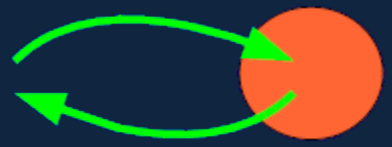
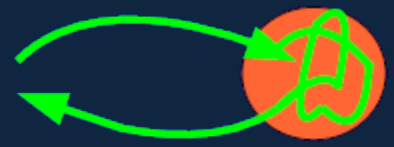


$G_0 V G_0$



$G_0 T G_0$

Getting *G*: Multiple Scattering

$$G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$$

Getting *G*: Multiple Scattering

$$G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$$

Central atom contrib.

$$G_c = G_0 + G_0 t_c G_0$$

EXAFS

$$G = G_c + G_c \sum_{i \neq c} t_i G_c + G_c \sum_{i \neq c} \sum_{j \neq c} t_i G_0 t_j G_c + \cdots$$

Getting *G*: Multiple Scattering

$$G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$$

Central atom contrib.

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EXAFS

$$G = G_c + G_c \sum_{i \neq c} t_i G_c + G_c \sum_{i \neq c} \sum_{j \neq c} t_i G_0 t_j G_c + \cdots$$

Graphically: Path expansion

Getting *G*: Full Multiple Scattering

$$G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$$

Getting *G*: Full Multiple Scattering

$$G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$$

Total scatt. matrix

$$T^{ij}_{LL'} = t^i_{LL'} \delta_{ij}$$

$$G = G^0 + G^0 T G^0 + G^0 T G^0 T G^0 + \ldots$$

Getting *G*: Full Multiple Scattering

$$G = G^0 + \sum_i G^0 t_i G^0 + \sum_{i \neq j} G^0 t_i G^0 t_j G^0 + \ldots$$

Total scatt. matrix

$$T^{ij}_{LL'} = t^i_{LL'} \delta_{ij}$$

$$G = G^0 + G^0 T G^0 + G^0 T G^0 T G^0 + \ldots$$

Sum and invert

XANES

$$G = \left[1 - G^0 T\right]^{-1} G^0$$

Implementation: FEFF Code

PHYSICAL REVIEW B VOLUME 58, NUMBER 12 15 SEPTEMBER 1998-II

Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure

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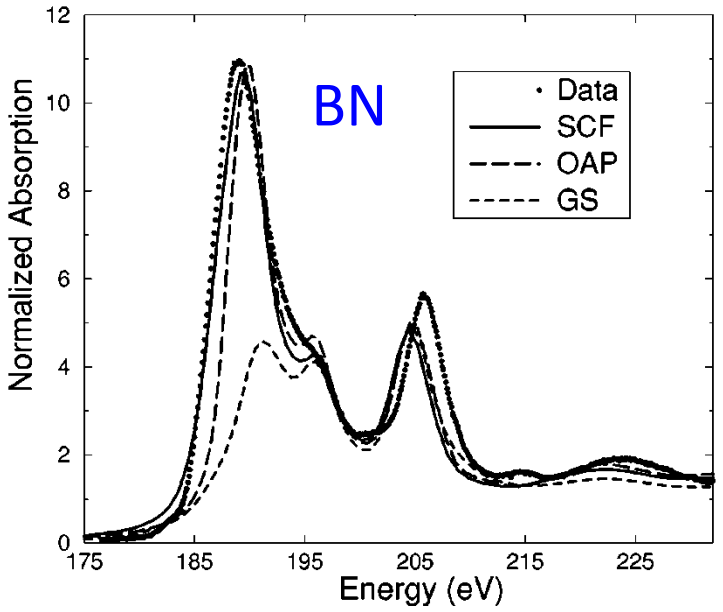
89 atom cluster



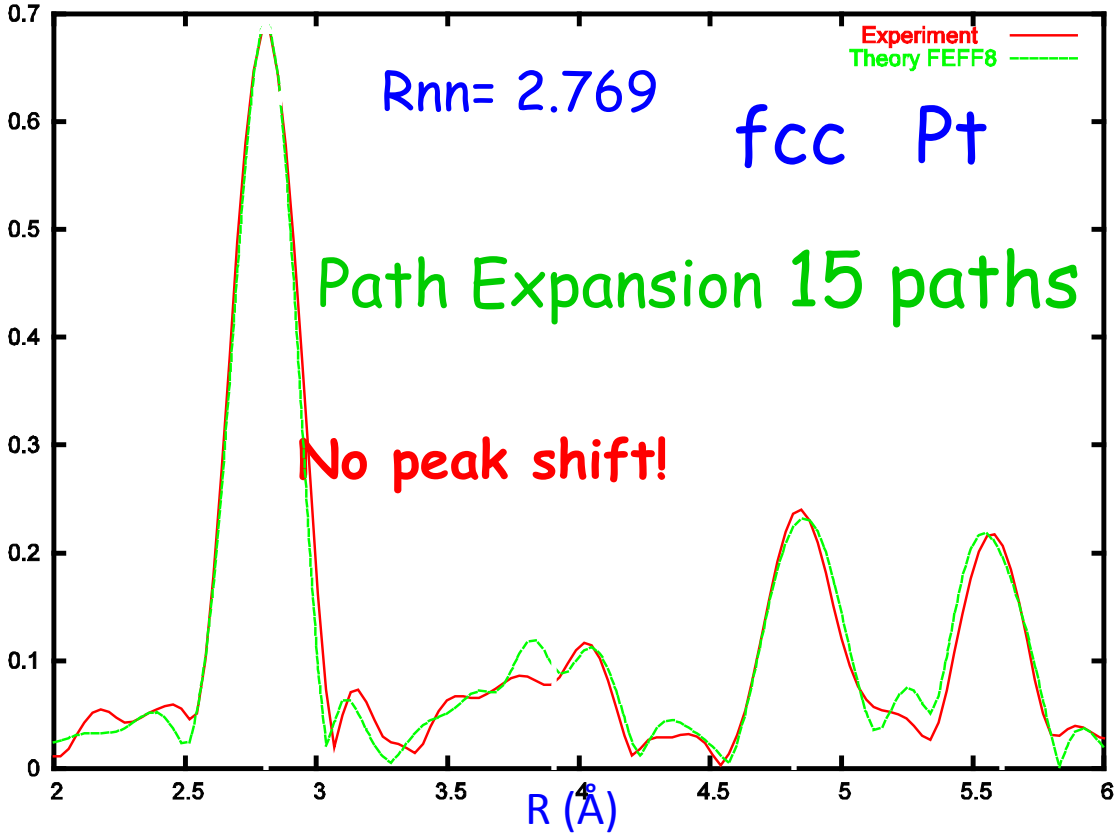
Core-hole, SCF potentials

Essential!

Example: Pt EXAFS – path expansion

Phase Corrected EXAFS Fourier Transform *

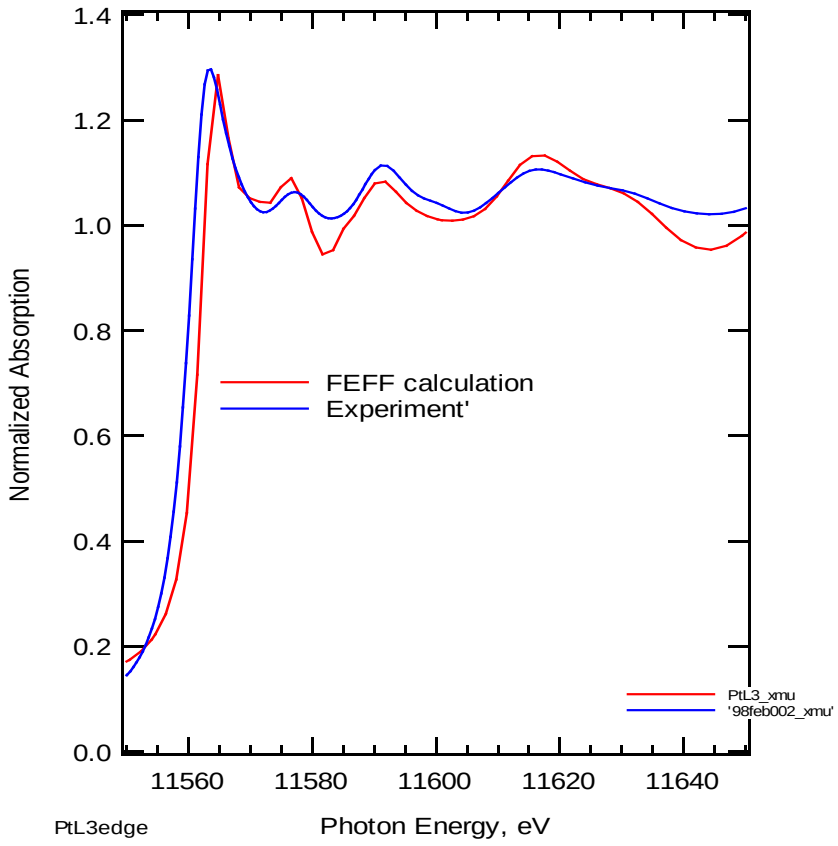
$\chi(R)$



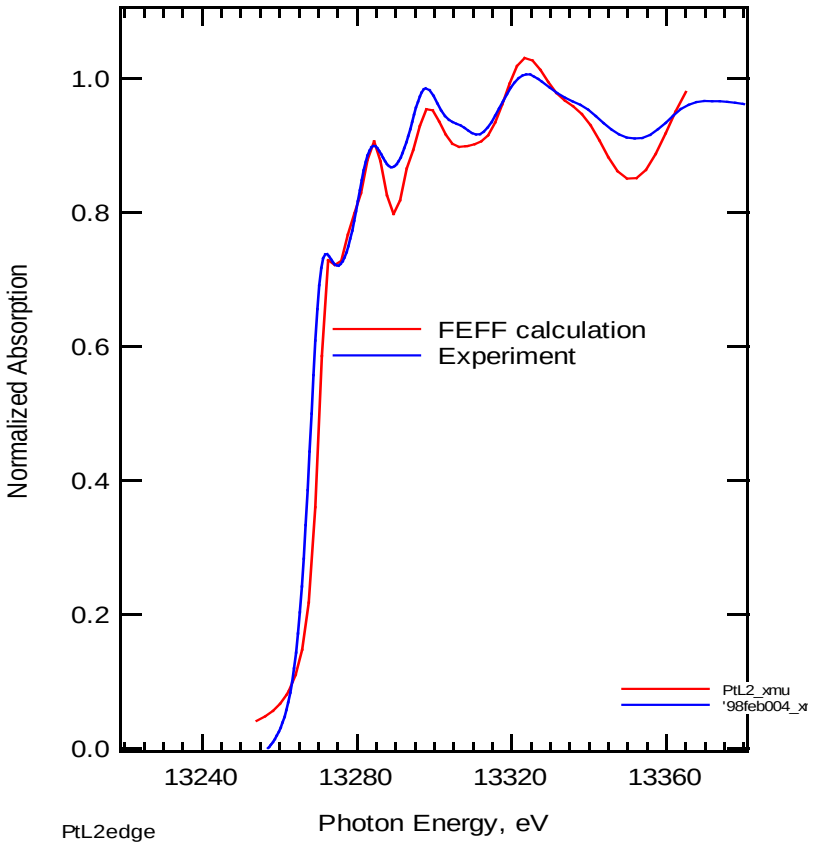
Theoretical phases accurate distances to < 0.01 Å

Example: Pt XANES full multiple-scattering

Pt L_3-edge



Pt L_2-edge **(S. Bare, UOP)**



- *Relativistic* FEFF8 code reproduces all spectral features, *including absence of white line at L_2-edge*.
- *Self-consistency essential*: position of Fermi level strongly affects white line intensity.

Green's Functions and Parallel Computation

PHYSICAL REVIEW B, VOLUME 65, 104107

Parallel calculation of electron multiple scattering using Lanczos algorithms

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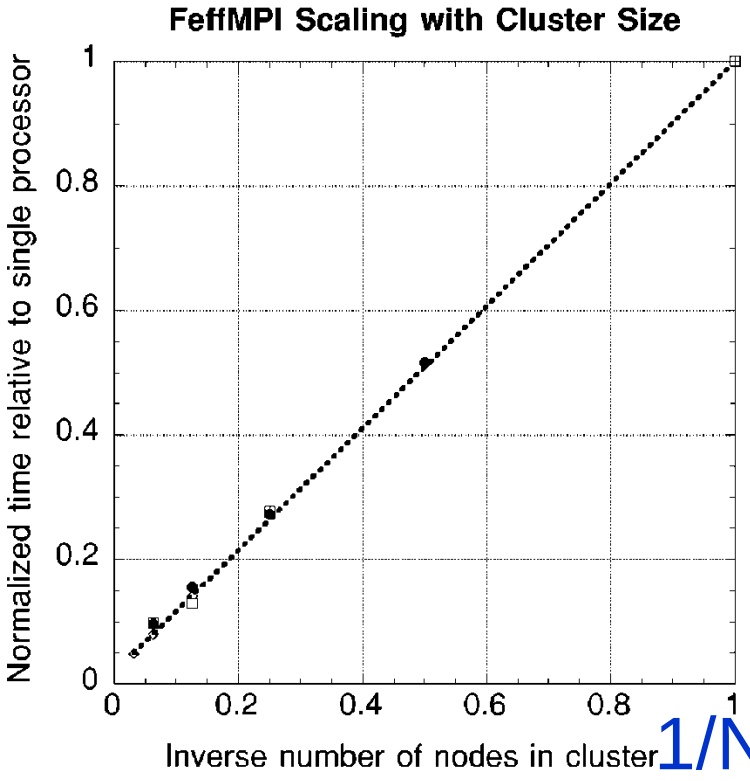
[2]*National Institute of Standards and Technology, Gaithersburg, Maryland 20899*



$1/N_{CPU}$

$$\mu(E) \sim -\tfrac{1}{\pi}\mathrm{Im}\,\langle \mathrm{i}|\,\hat{\epsilon}\cdot\mathbf{r}'\,\mathrm{G}(\mathbf{r}',\mathbf{r},\mathrm{E})\,\hat{\epsilon}\cdot\mathbf{r}\,|\mathrm{i}\rangle$$

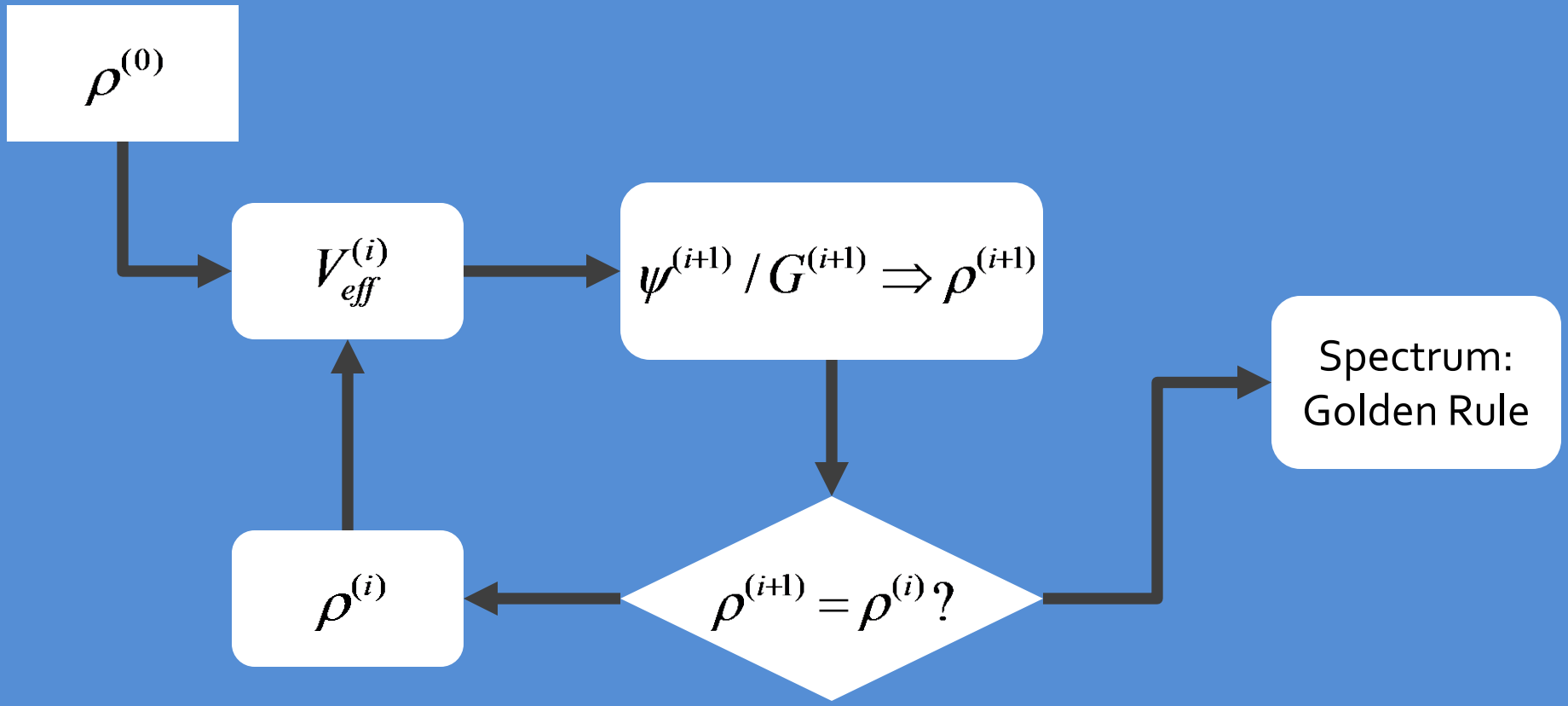
Energy E
is just a parameter !

"Natural parallelization"

Each CPU does one energy

Self-consistent Densities and Potentials

$$\rho(r) = -\frac{1}{\pi}\int_{-\infty}^{E_{Fermi}} \mathrm{Im}[G(r,r;E)]\,dE$$



Key approximations in FEFF

Dirac-Fock relativistic atomic states ;
semi-relativistic scattering states

Spherical overlapped muffin-tin potentials:
Huge simplification of the problem

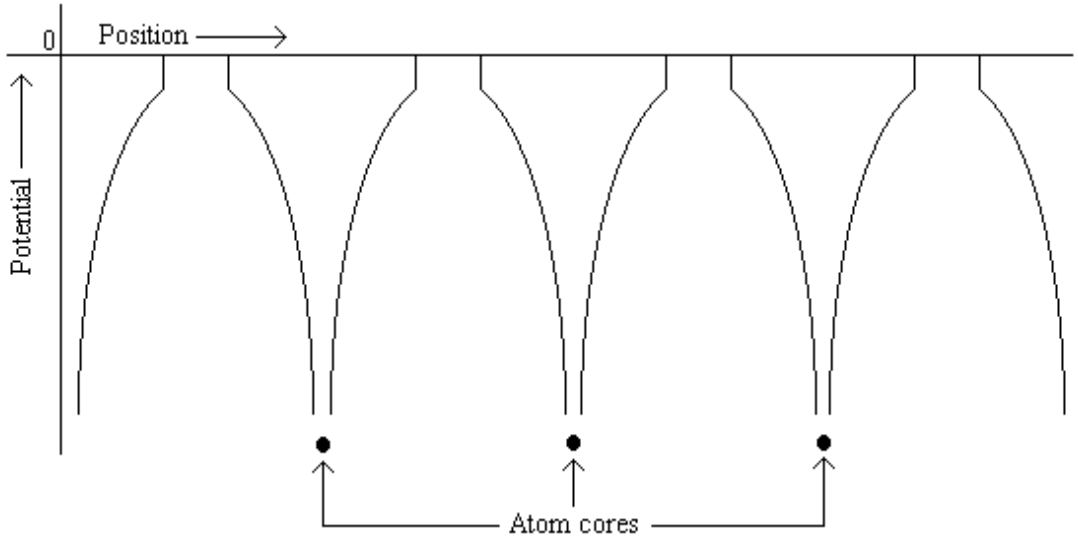
Quasi-particle approximation:
Electron propagates in lossy medium described by
Approximate self-energy

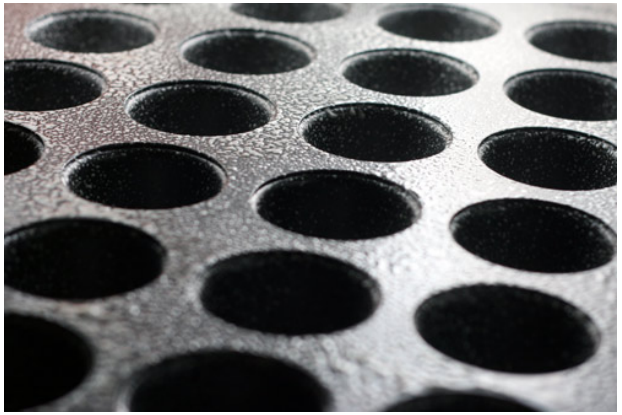
Core-hole treatment:
RPA or DFT-Screened core-hole

The muffin-tin potential

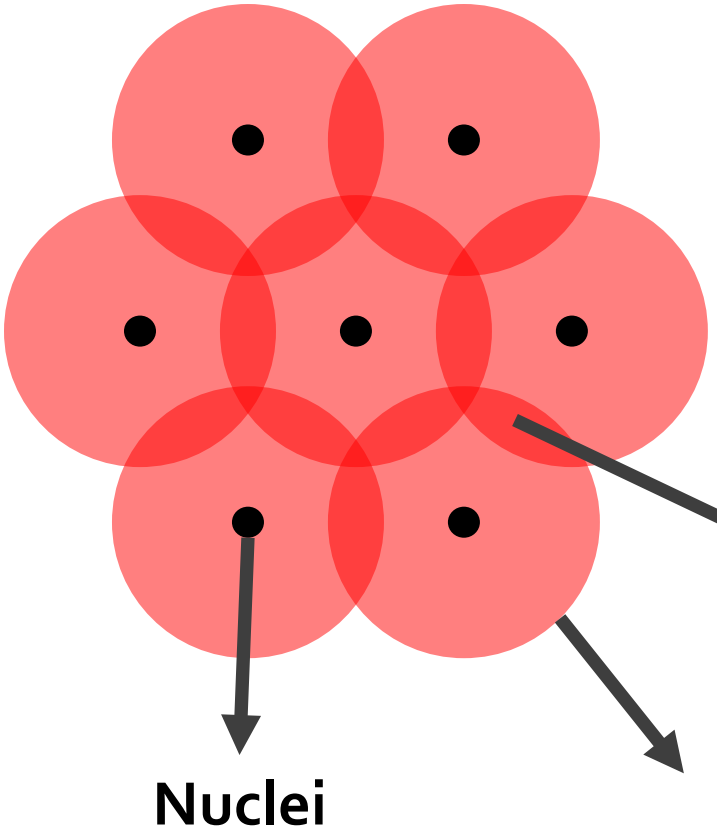
Scattering potential partition into muffin-tins

$$V = \sum_i v_i$$





The overlapped muffin-tin potential (~ 10%)



Improved density:

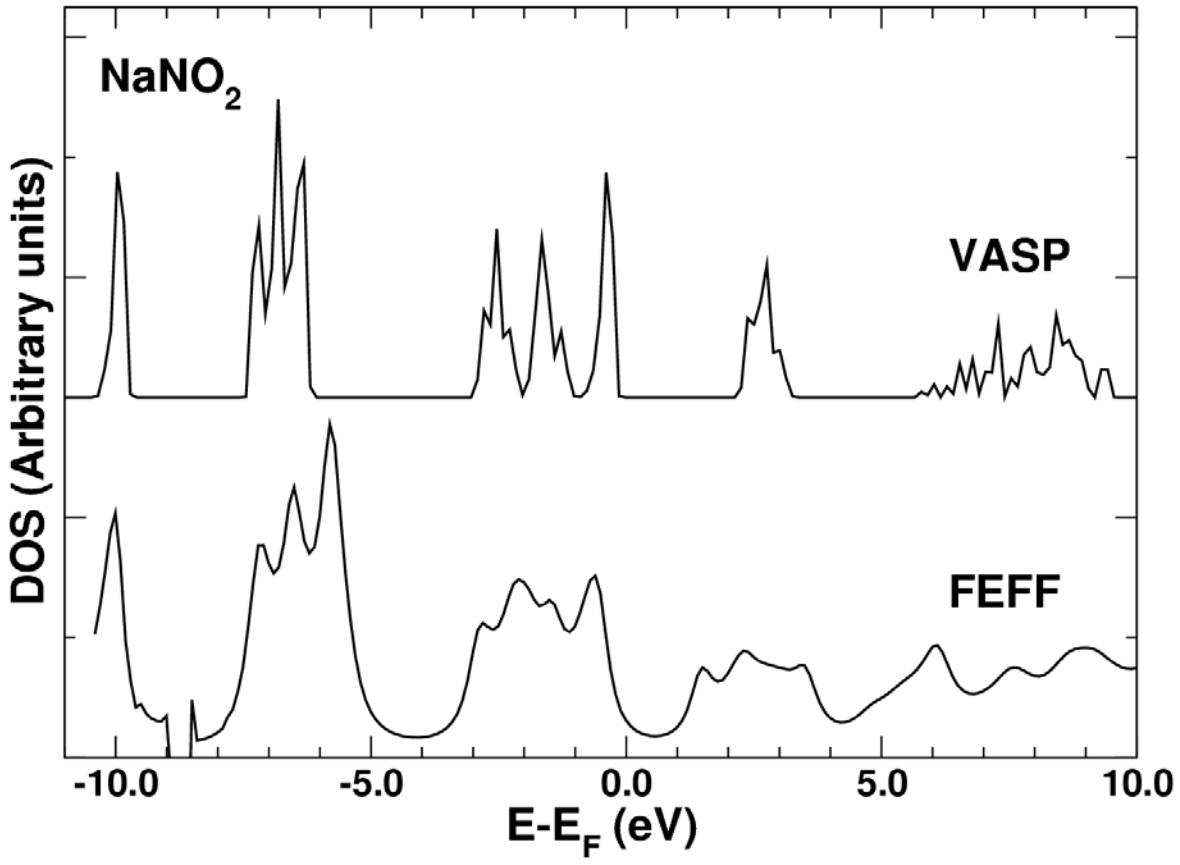
Resembles "bonding"

Charge redistribution

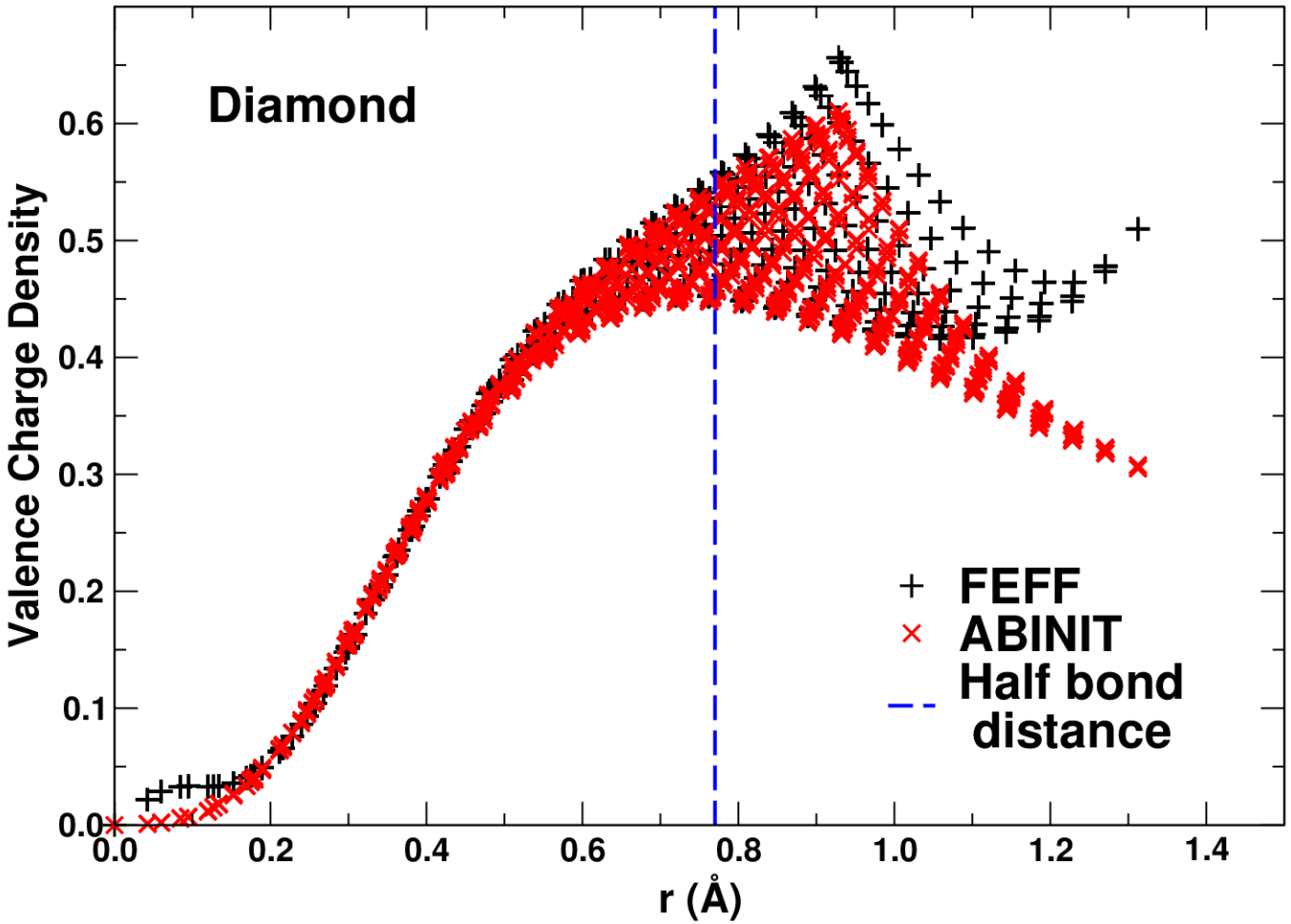
Charge neutrality built in

? Spherical approximation ?

FEFF Density of States vs full potential codes



FEFF electron density in real space vs full potential codes



Disorder and Debye-Waller factors

DW factors:

- Crucial for EXAFS
- Very little effect in XANES region
- Can be included anyway in single-scattering approx.
- Both *ab initio* and model forms

Static Disorder:

- May be important in XANES
- Need external input for FEFF simulations
- Methods MD trajectories, MC sampling …

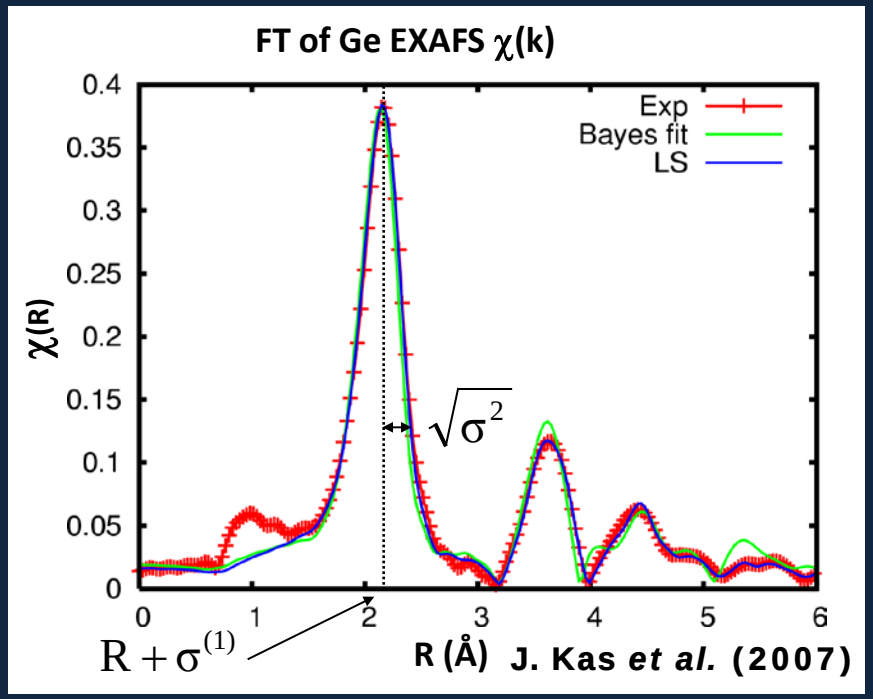
Quick intro to DW factors

Multiple Scattering Path XAFS DW Factor

Average commonly expressed in terms of the cumulant expansion

$$\left\langle e^{i2kr} \right\rangle \equiv e^{2ikR_0} e^{-W(T)}$$

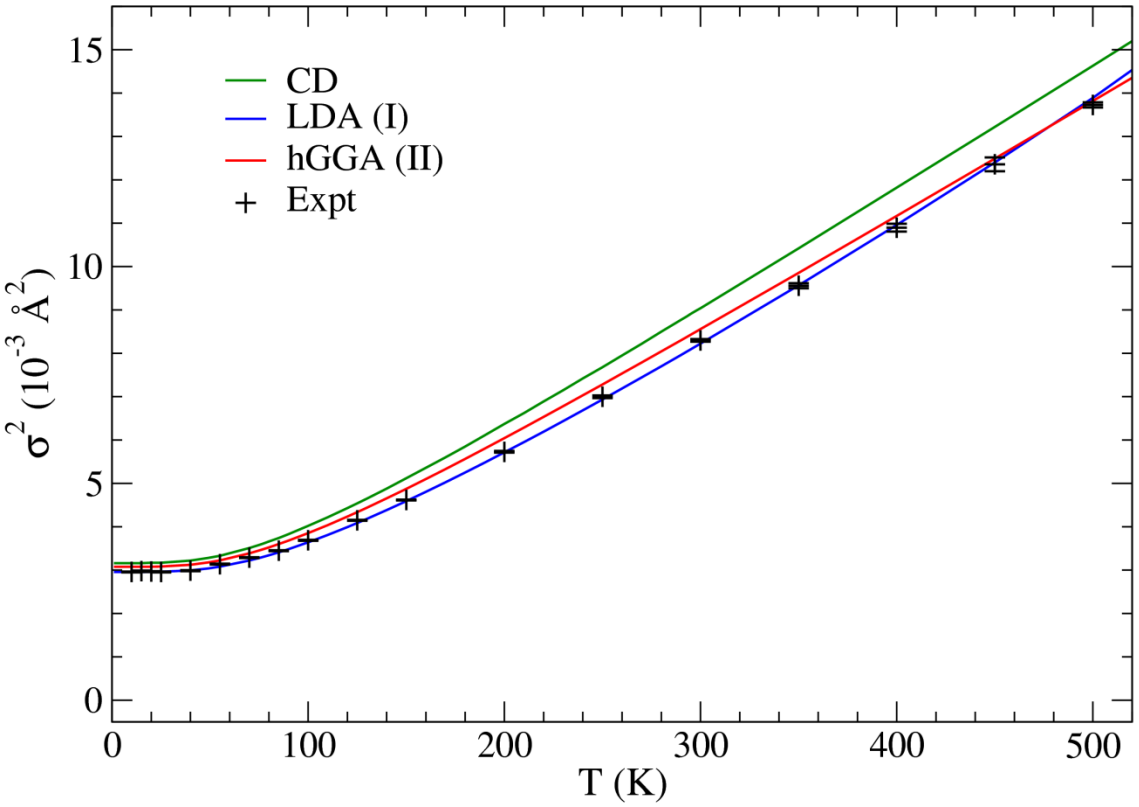
$$W(T) = -\sum_{n=1}^{\infty} \frac{(2ik)^n}{n!} \sigma^{(n)}(T)$$



Leading cumulants

$$\begin{cases} \sigma^{(1)} = \langle r - R_0 \rangle \\ \sigma^{(2)} = \left\langle (r - \bar{r})^2 \right\rangle \equiv \sigma^2(T) \\ \sigma^{(3)} = \left\langle (r - \bar{r})^3 \right\rangle \end{cases}$$

EXAFS near-neighbor DW Factor of Cu



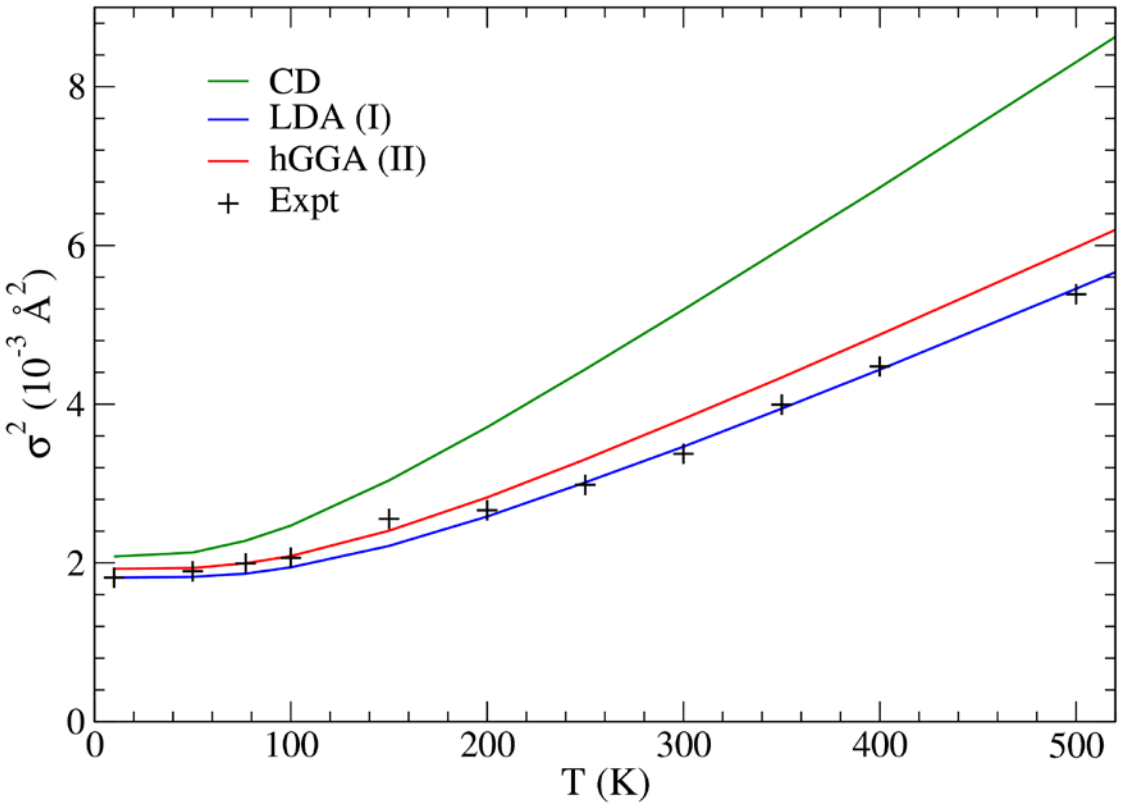
CD (Correlated Debye):
Standard FEFF

LDA, hGGA:
Ab initio DW

Isotropic bonding:
Good CD results

Expt: Fornasini et al. (2004)

EXAFS near-neighbor DW Factor of Ge



CD (Correlated Debye):
Default in FEFF

LDA, hGGA:
Ab initio DW

Directional bonding:
Needs AIDW

Expt: Dalba et al. (1999)

Ab Initio DW factors: Lanczos algorithm

XAFS DW Factor for path R:

$$\sigma_R^2(T) = \frac{\hbar}{2\mu_R}\int_0^\infty \frac{1}{\omega}\coth\left(\frac{\beta\hbar\omega}{2}\right)\rho_R(\omega)\,d\omega$$

VDOS expressed as imaginary part of the phonon propagator

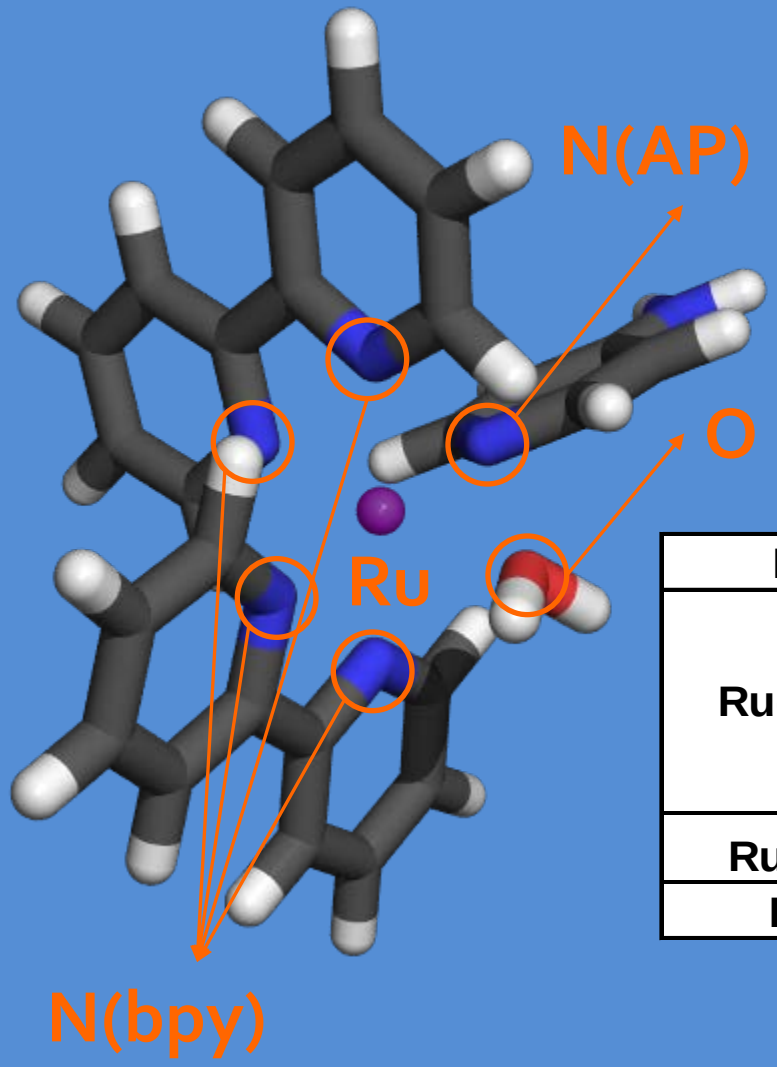
$$\rho_R(\omega) = -\frac{2\omega}{\pi}\mathrm{Im}\left\langle 0\right|\frac{1}{\omega^2 - \mathbf{D} + i\varepsilon}\left|0\right\rangle$$

Seed state: Displacement along path

Dynamical Matrix: Calculated using ab initio methods (Abinit, Gaussian, VASP, etc)

Ab Initio DW Factors in Metal-Ligand Complexes

$Ru(bpy)^2(AP)(H_2O)^{++}$



Good agreement for tight ligands (bpy)

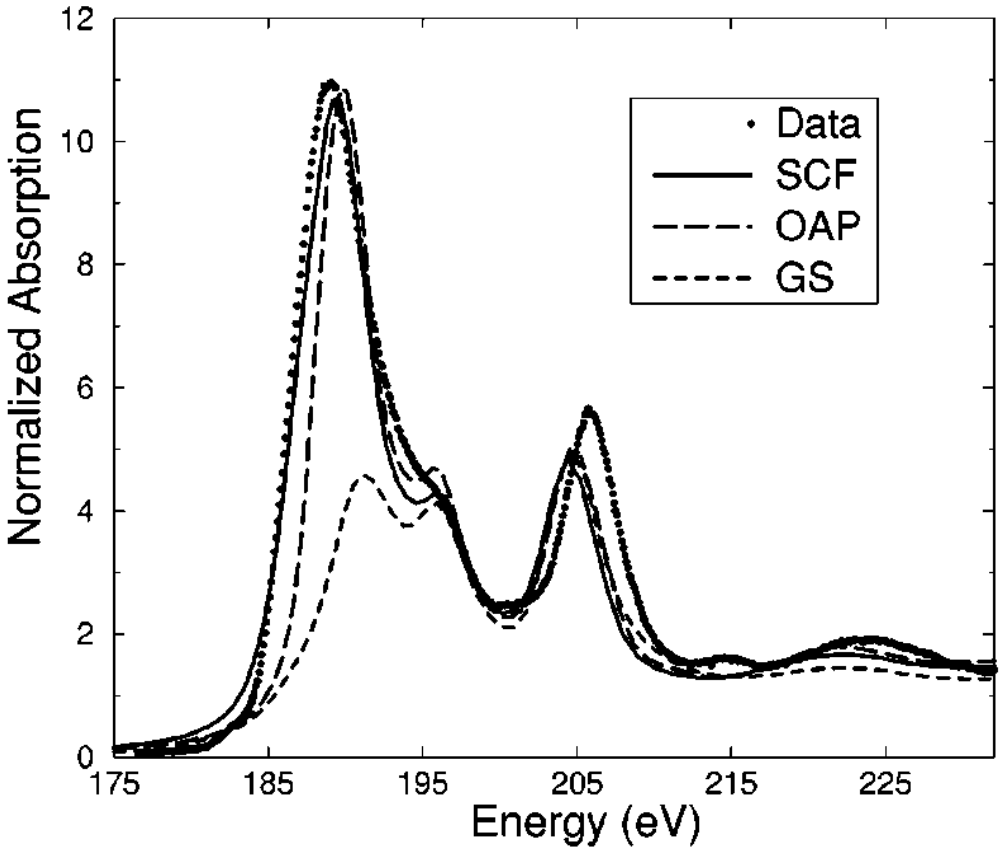
Useful agreement for weak ligands (AP and H_2O)
Still within error margin

	R_{M-L} (in Å)		σ^2 (in 10^{-3} Å^2)	
Path	Theory	Exp	Theory	Exp.
Ru-N(bpy)	2.08 2.04 2.10 2.09	2.05±0.01	2.49 2.32 2.60 2.50	2.6±0.9
Ru-N(AP)	2.14	2.10±0.03	2.61	4±3
Ru-O	2.22	2.06±0.05	4.93	9±7

Expt: Salassa et al., J. of Physics: Conference Series 190, 012141 (2009)

Beyond DFT: Quasi-particle Self-Energy Effects

Quasi-particle (QP) effects: $G = [E - H - \Sigma]^{-1}$



BN 89 atom cluster

Ground state potential:

Usually insufficient

Need QP effects

and SCF potentials

Improvements to the theory: key many body effects
Lecture III. Inelastic losses and Manybody effects

Treatment of the core hole:

- Screening DFT or RPA
- Chemical shifts

Self-energy approximations:

- Need more than single-pole self-energy

Many-body effects:

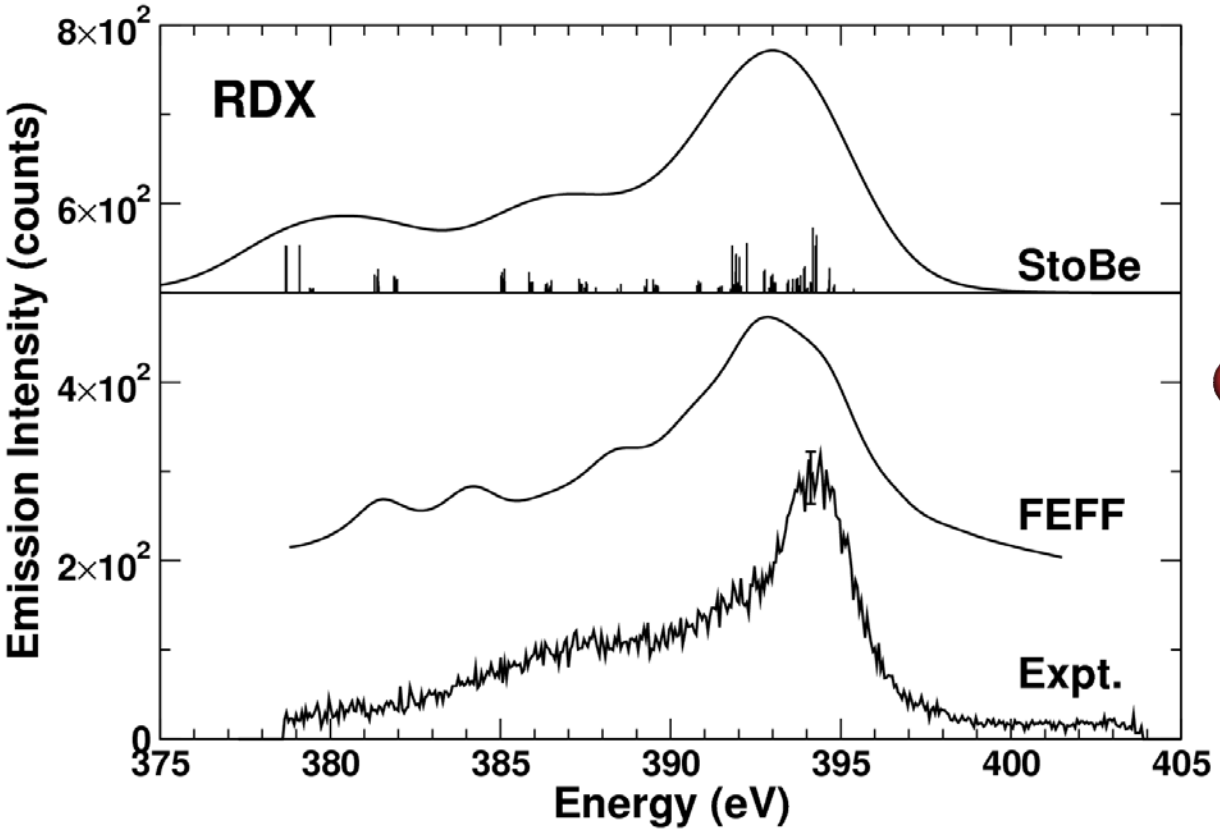
- Multi-electron excitations S_0^2
- Charge transfer excitations:

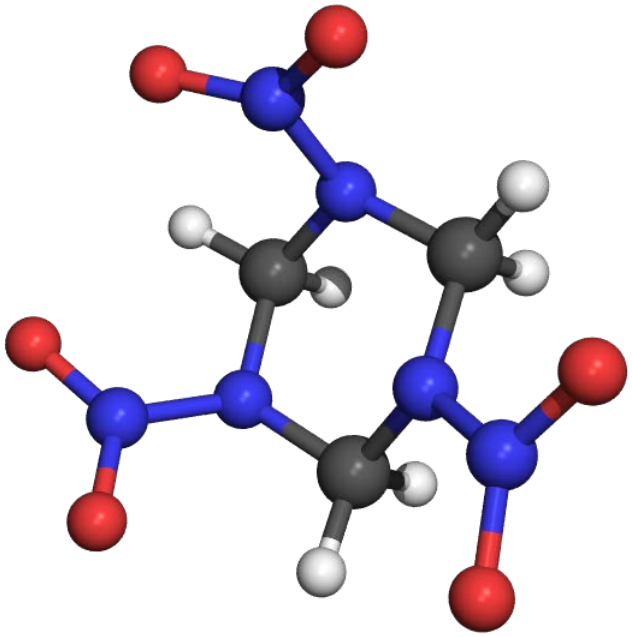
Other FEFF capabilities

Quick overview of other FEFF capabilities:

- XES
- RIXS
- Compton Profiles
- Reciprocal space: EELS and impurity GF
- Hubbard U method

Non-resonant X-ray Emission (XES)





RDX
(High explosive)

Vila et al., J. Phys. Chem. A 2011, 115, 3243

Resonant Inelastic X-ray Scattering (RIXS)

PHYSICAL REVIEW B 83, 235114 (2011)

Real-space Green's function approach to resonant inelastic x-ray scattering

J. J. Kas,[1] J. J. Rehr,[1,*] J. A. Soininen,[2] and P. Glatzel[3]
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[2]*Department of Physics, P.O. Box 64, University of Helsinki, FI-00014 Helsinki, Finland*
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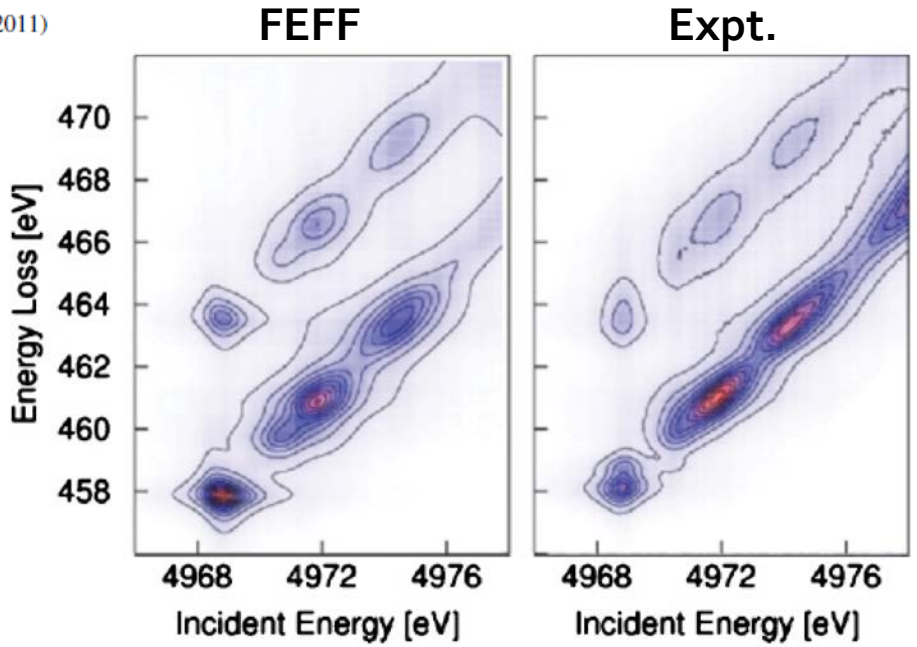
(Received 21 January 2011; revised manuscript received 7 April 2011; published 8 June 2011)

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{\omega}{\Omega}\sum_F \left| \frac{\sum_M \langle F|\Delta_2^\dagger|M\rangle\langle M|\Delta_1|\Psi_0\rangle}{E_M - \Omega - E_0 + i\Gamma_M} \right|^2 \times \delta(\Omega - \omega + E_0 - E_F)$$

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \frac{\omega}{\Omega}\int d\omega_1 \frac{\mu_e(\omega_1)\mu(\Omega - \omega - \omega_1 + E_b)}{|\omega - \omega_1 - i\Gamma_b|^2}$$

TiO_2 (Ti Kα)



Compton Profiles

PHYSICAL REVIEW B **85**, 115135 (2012)

Real-space Green's function calculations of Compton profiles

Brian A. Mattern, Gerald T. Seidler,* Joshua J. Kas, Joseph I. Pacold, and John J. Rehr
Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA
(Received 2 February 2012; revised manuscript received 16 March 2012; published 29 March 2012)

PHYSICAL REVIEW B **94**, 214201 (2016)

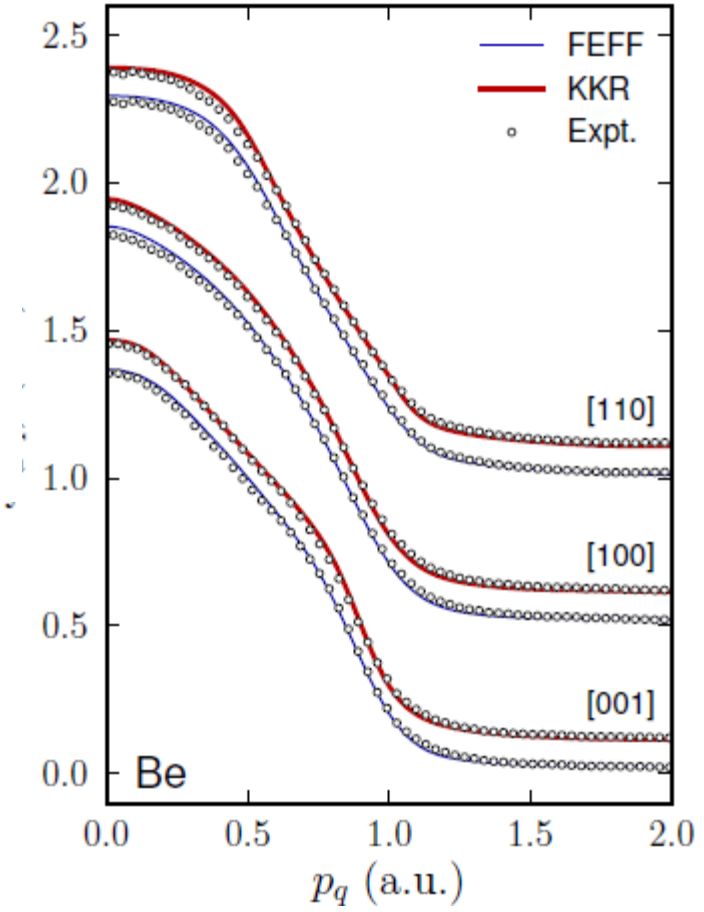
Finite-temperature calculations of the Compton profile of Be, Li, and Si

E. Klevak, F. D. Vila, J. J. Kas, J. J. Rehr, and G. T. Seidler
Department of Physics, University of Washington, Seattle, Washington 98195, USA
(Received 3 August 2016; published 2 December 2016)

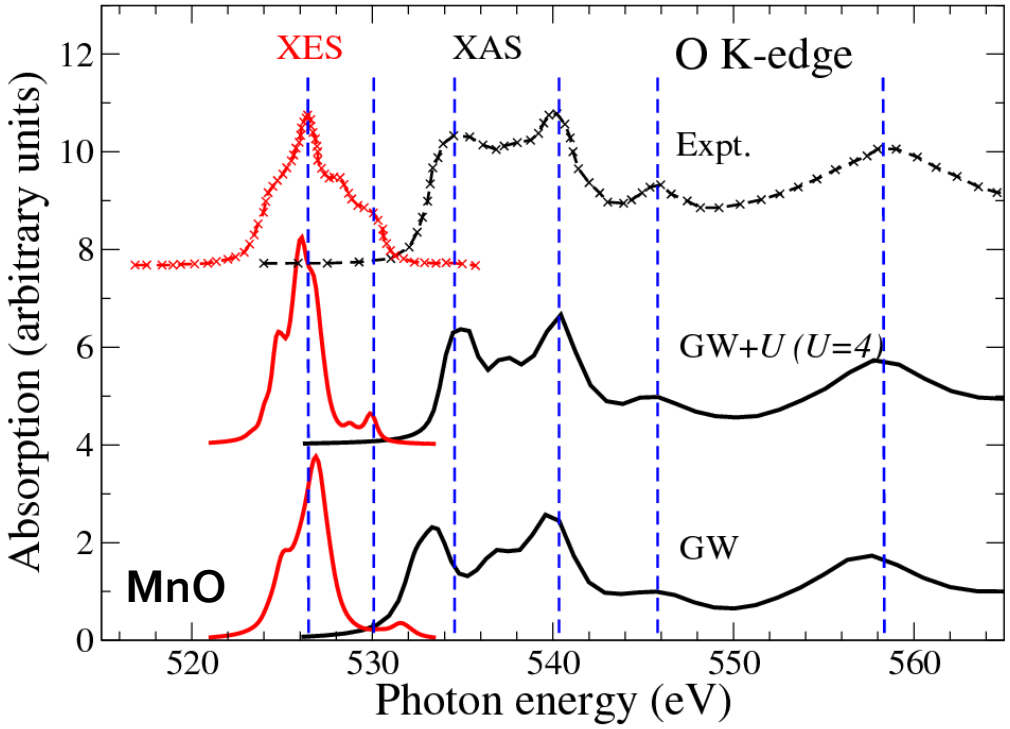
$$S(\mathbf{q},\omega) = \sum_F \left| \langle F | \sum_j \exp(i\mathbf{q}\cdot\mathbf{r}_j) | I \rangle \right|^2 \delta(E_F - E_I - \hbar\omega)$$

$$S(\mathbf{q},\omega) = (m/\hbar q) J(p_q)$$

$$J(p_q) \equiv \int d^3p \rho(\mathbf{p}) \delta(p_q - (\omega m/q - \hbar q/2))$$

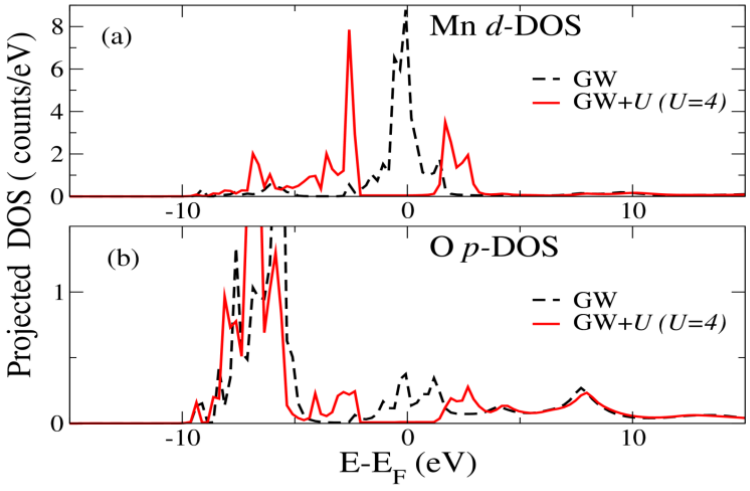


Strongly correlated systems: Hubbard GW+U



U calculated using
constrained RPA within RSMS

(Nearly) parameter free



Phys. Rev. B 85 165123 (2012)

Further information

The FEFF Project website:

URL: feffproject.org

The FEFF Users Guide:

URL: feffproject.org/feffproject-feff-documentation.html

Developers contact:

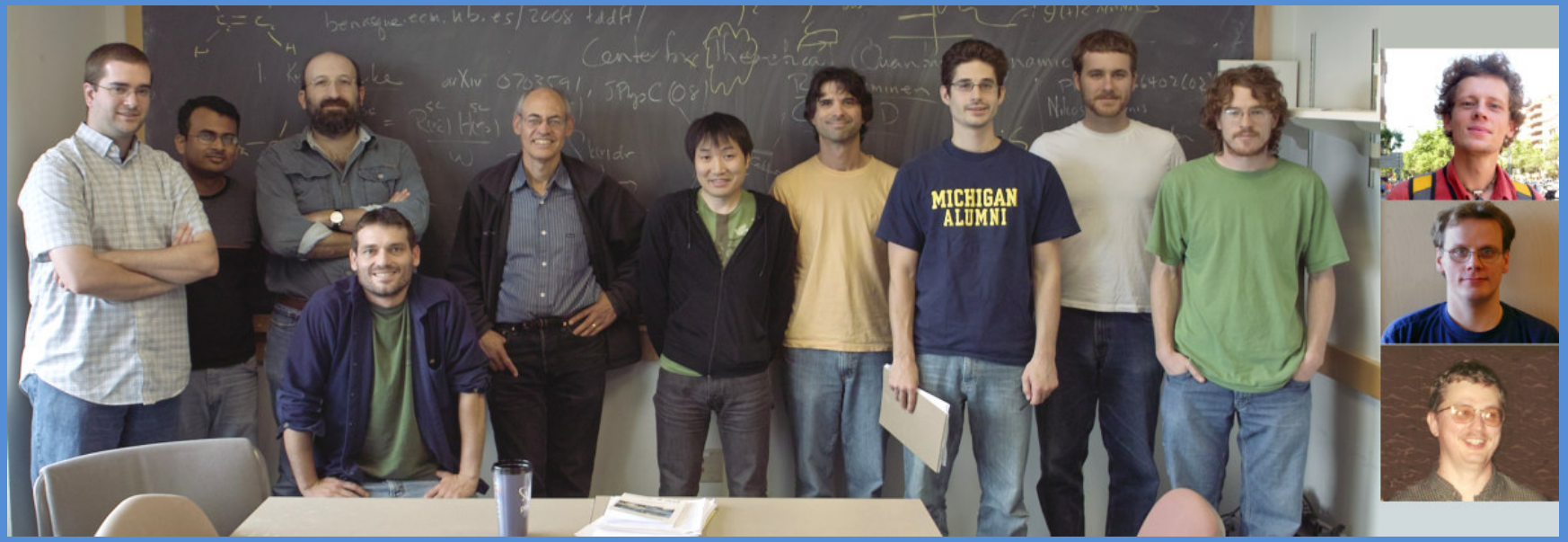
URL: feffproject.org/feffproject-contact.html

Summary

Take away messages

Know the basics of RSMS/RSGF theory
Understand the key approximations in FEFF
Know some of FEFF's advanced capabilities

Acknowledgments: the FEFF group



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