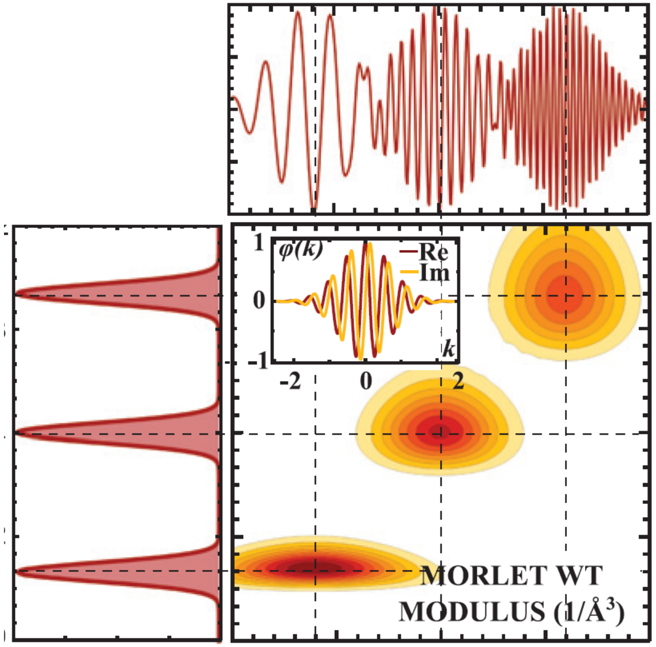
Wavelet analysis of EXAFS spectra



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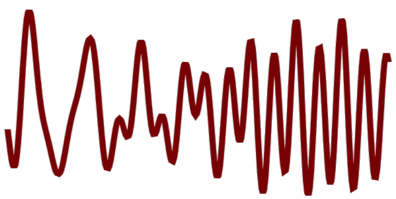
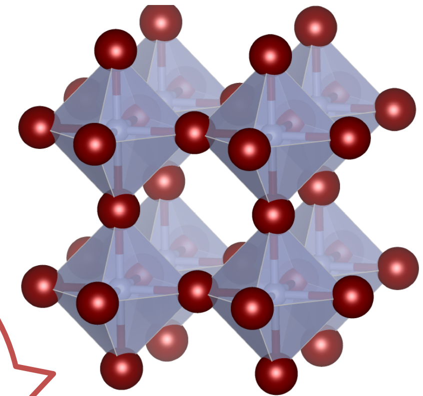
EXAFS data analysis

Experimental EXAFS



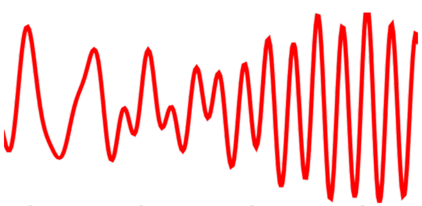
Initial structure model



Comparison

Model refinement

Theoretical EXAFS



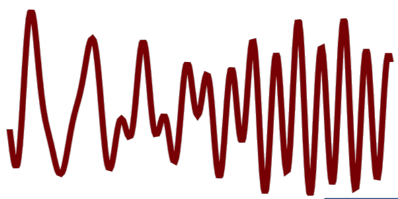
EXAFS modeling

$$\chi(k) = \sum_p \chi_p(k)$$

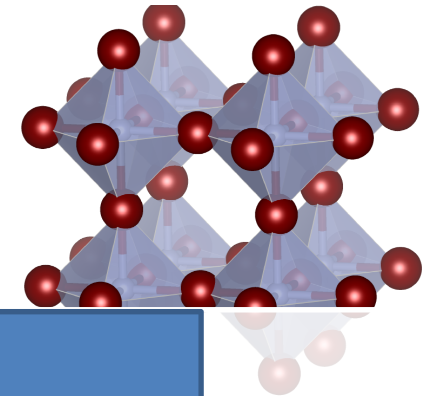
$$\chi_p(k) = S_0^2 \int_0^{+\infty} \boldsymbol{g_p}(\boldsymbol{R}) \frac{f_p(k,R)}{kR^2} \sin\left(2kR + \phi_p(k)\right) dR$$

EXAFS data analysis

Experimental EXAFS



Initial structure model



How to construct /choose the initial structure model?

Comparison

Theoretical EXAFS

EXAFS modeling

$$\chi(k) = \sum_p \chi_p(k)$$

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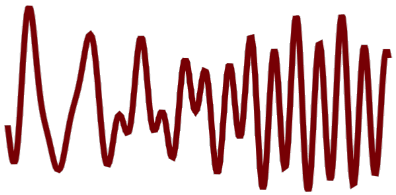
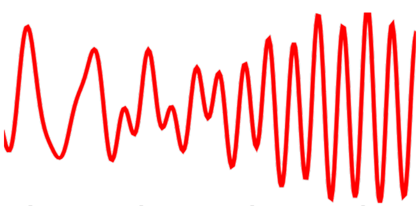
EXAFS data analysis

Experimental EXAFS



Comparison

Theoretical EXAFS



How to compare theoretical and experimental data?

Initial structure model

EXAFS modeling

$$\chi(k) = \sum_p \chi_p(k)$$

$$\chi_p(k) = S_0^2 \int_0^{+\infty} \boldsymbol{g_p(R)} \frac{f_p(k,R)}{kR^2} \sin\left(2kR + \phi_p(k)\right) dR$$

Outline

- ❑Fourier-transform of EXAFS data
- ❑Short-time Fourier transform
- ❑Wavelet transform
- ❑Wavelet transform of EXAFS data: examples

Fourier transform

VOLUME 27, NUMBER 18 PHYSICAL REVIEW LETTERS 1 NOVEMBER 1971

New Technique for Investigating Noncrystalline Structures: Fourier Analysis of the Extended X-Ray–Absorption Fine Structure*

Dale E. Sayers† and Edward A. Stern†‡
Department of Physics, University of Washington, Seattle, Washington 98105

and

Farrel W. Lytle
Boeing Scientific Research Laboratories, Seattle, Washington 98124
(Received 16 July 1971)

$$\chi(k) = \sum_p \chi_p(k)$$

$$\chi_p(k) = S_0^2 \int_0^{+\infty} \boldsymbol{g_p(R)} \frac{f_p(k,R)}{kR^2} \sin\left(2kR + \phi_p(k)\right) dR$$

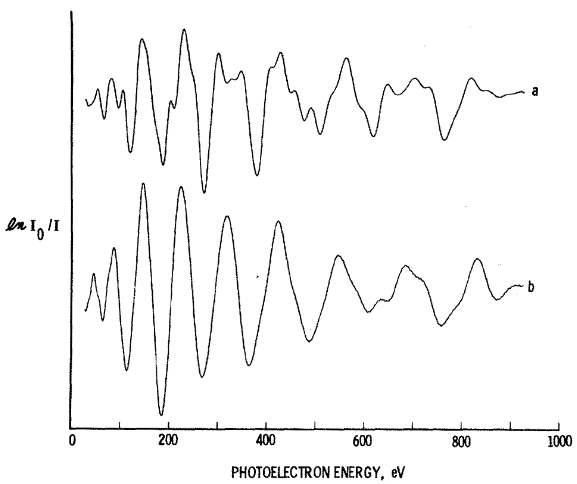


FIG. 1. Smoothed experimental EXAFS data for (a) crystalline and (b) amorphous Ge. Only the oscillatory part χ of the absorption edge is shown.

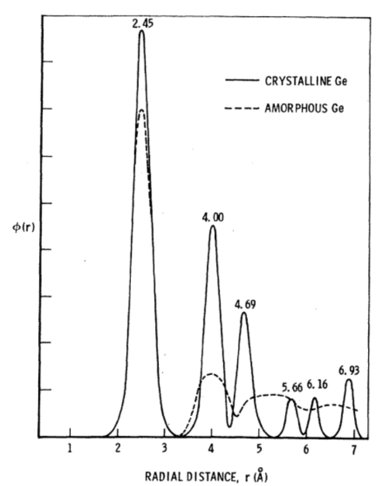


FIG. 2. Fourier transformation of the data of Fig. 1. $\varphi(r)$, a radial structure function, compares amorphous and crystalline Ge. Numbers over the peaks indicate the measured distances in Å.

Taking into account sinusoidal nature of EXAFS signal, **Fourier transform** seems to be a natural way to get quick first impression on material structure.

$$\mathrm{FT}_\chi(R) = (2\pi)^{-1/2} \int_{k_{\min}}^{k_{\max}} e^{2iRk} \chi(k) dk$$

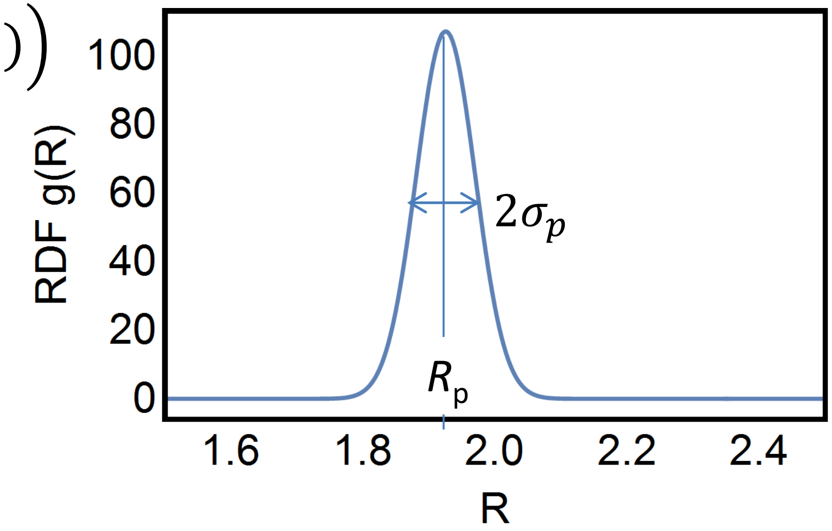
EXAFS equation

$$\chi(k) = \sum_p \chi_p(k)$$

$$\chi_p(k) = S_0^2 \int_0^{+\infty} \boldsymbol{g_p(R)} \frac{f_p(k,R)}{kR^2} \sin\left(2kR + \phi_p(k)\right) dR$$

$$\chi_p(k) = S_0^2 N_p \frac{f_p(k\,)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right)$$

For systems with small disorder (e.g., crystalline materials), harmonic approximation is usually adequate:

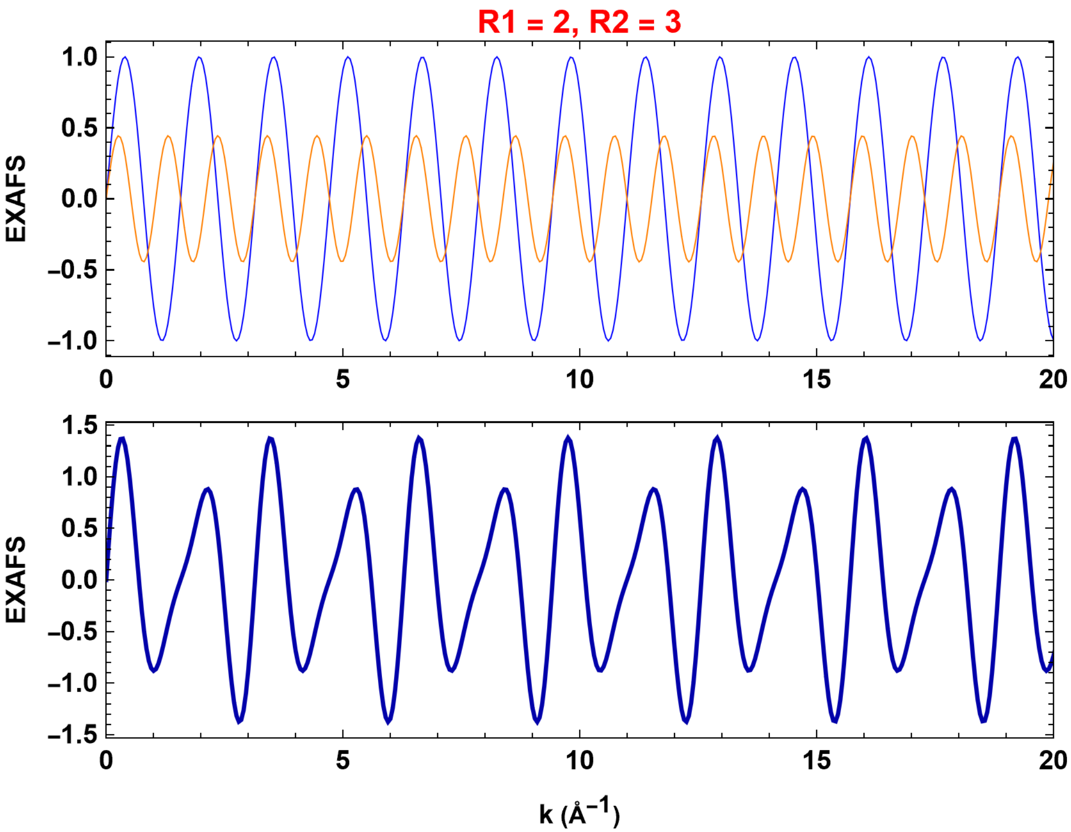


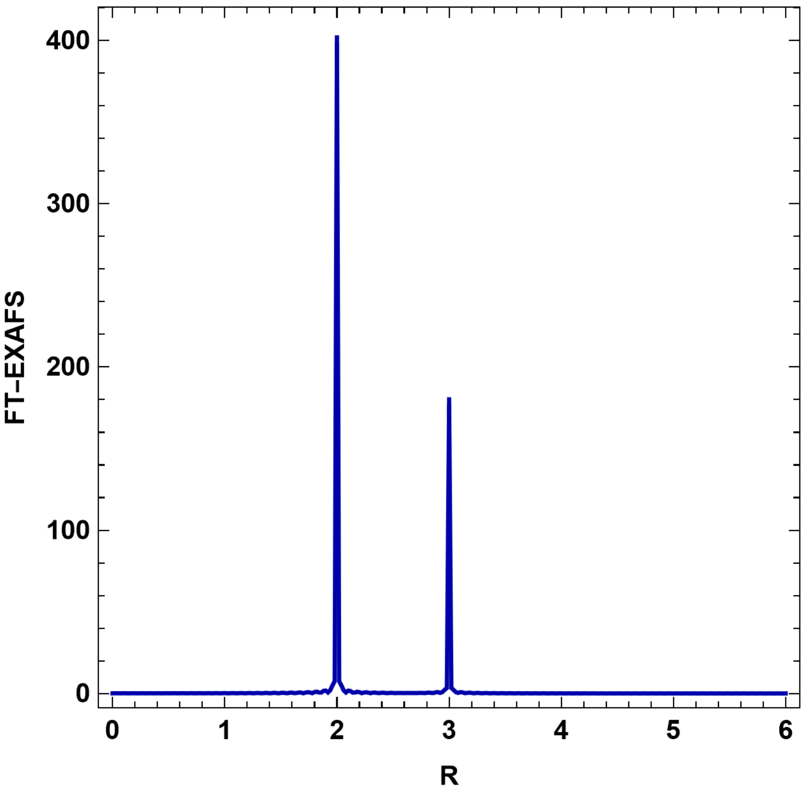
J. J. Rehr and R. C. Albers, Rev. Mod. Phys., 72 (2000).

Fourier transform: frequency

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p \sin(2kR_p)}{R_p^2}$$

$$FT_\chi(R) = (2\pi)^{-\frac{1}{2}} \int_{k_{min}}^{k_{max}} e^{2iRk} \chi(k) dk$$





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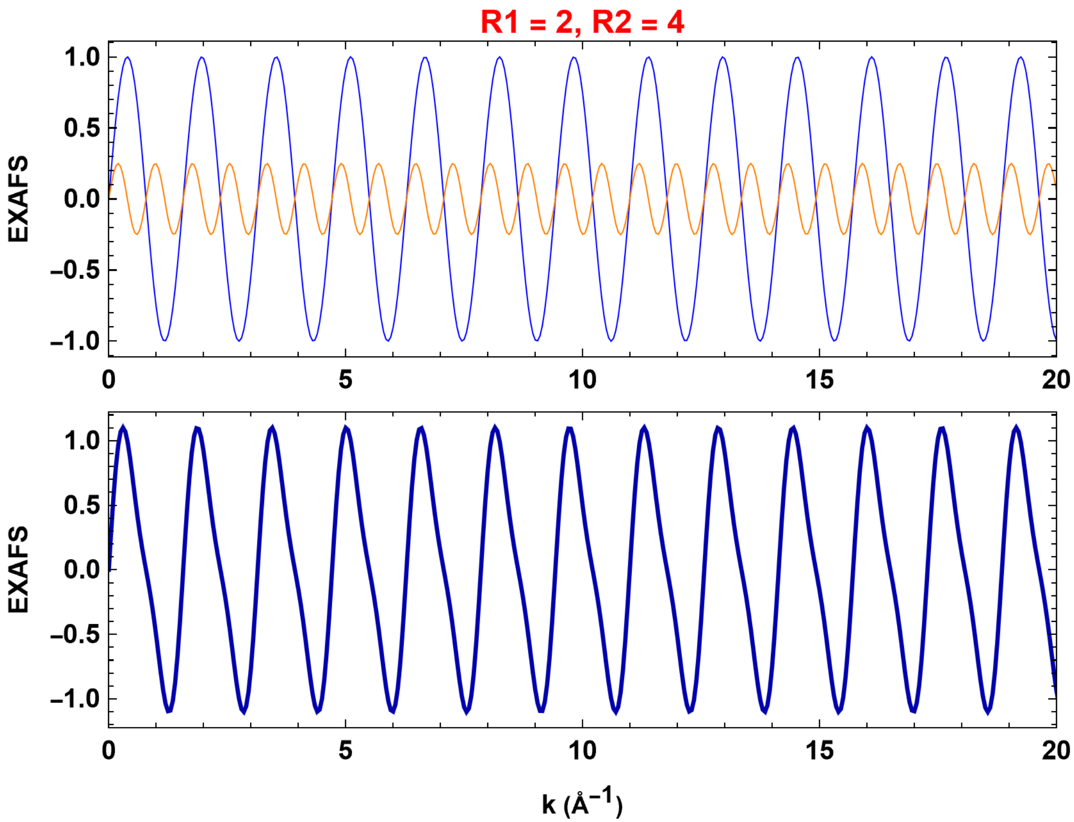

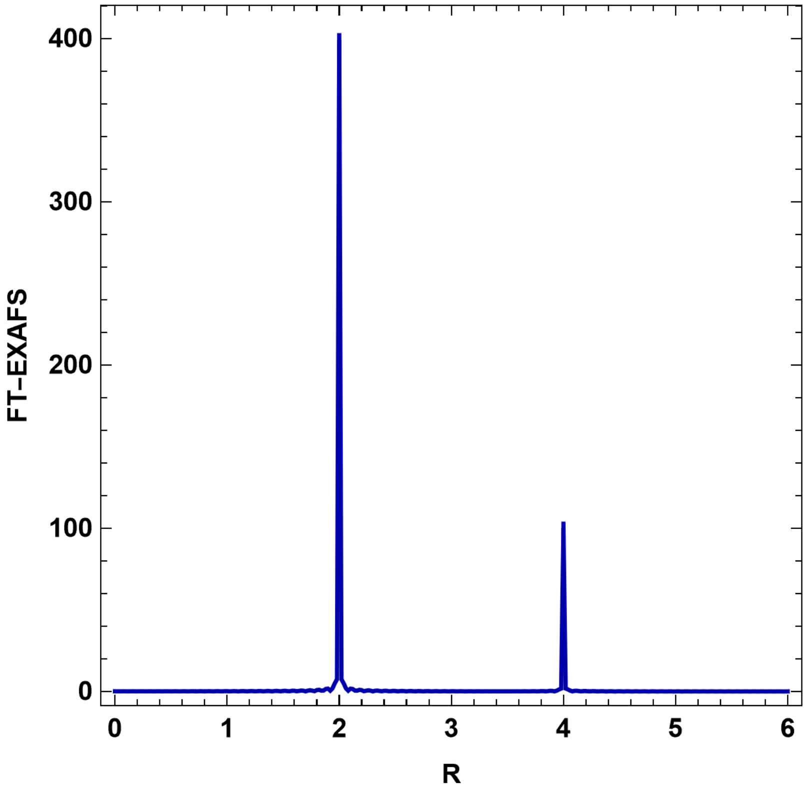

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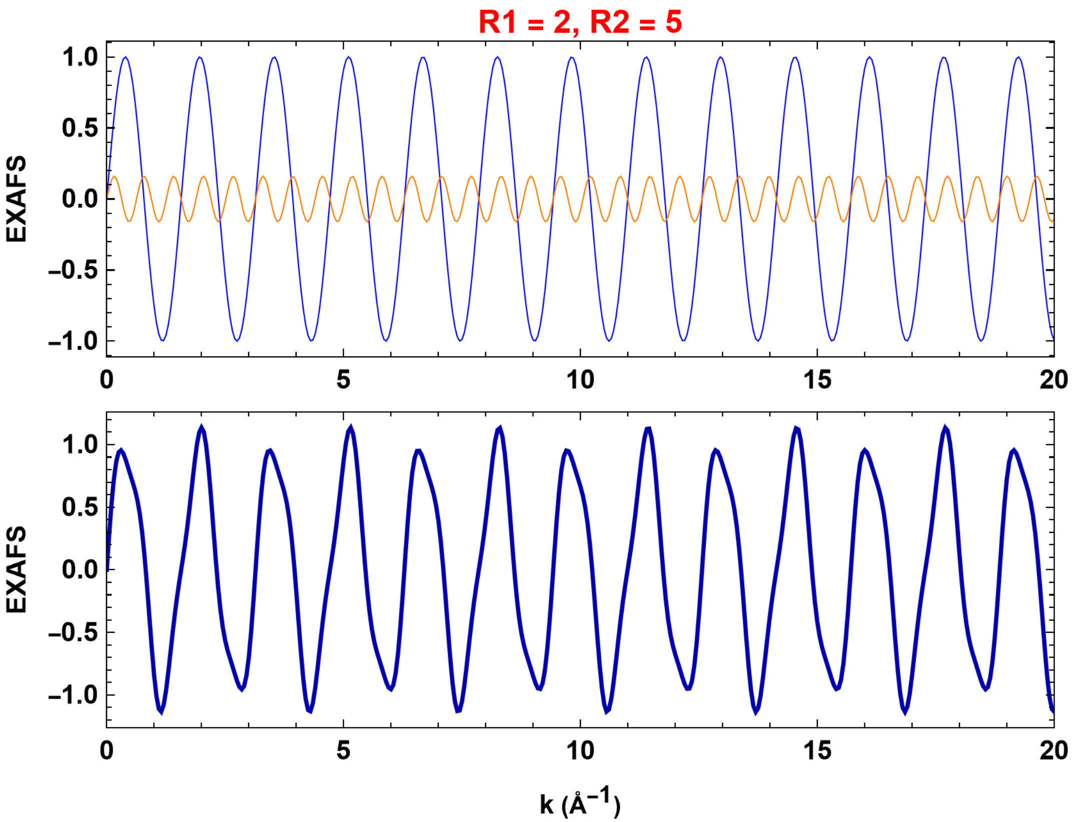

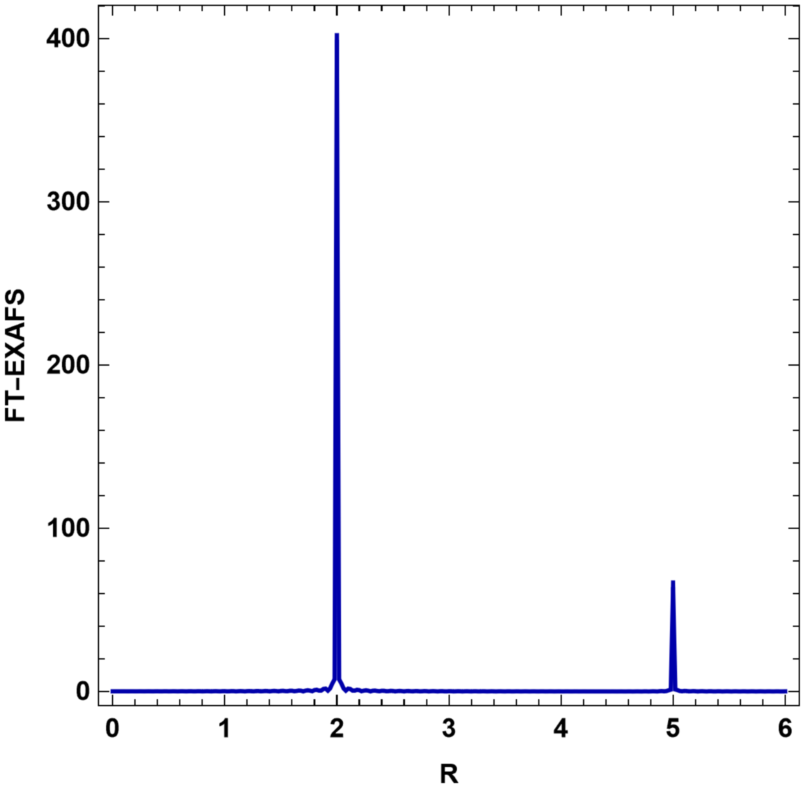

Fourier transform: signal length

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p \sin(2kR_p)}{R_p^2}$$

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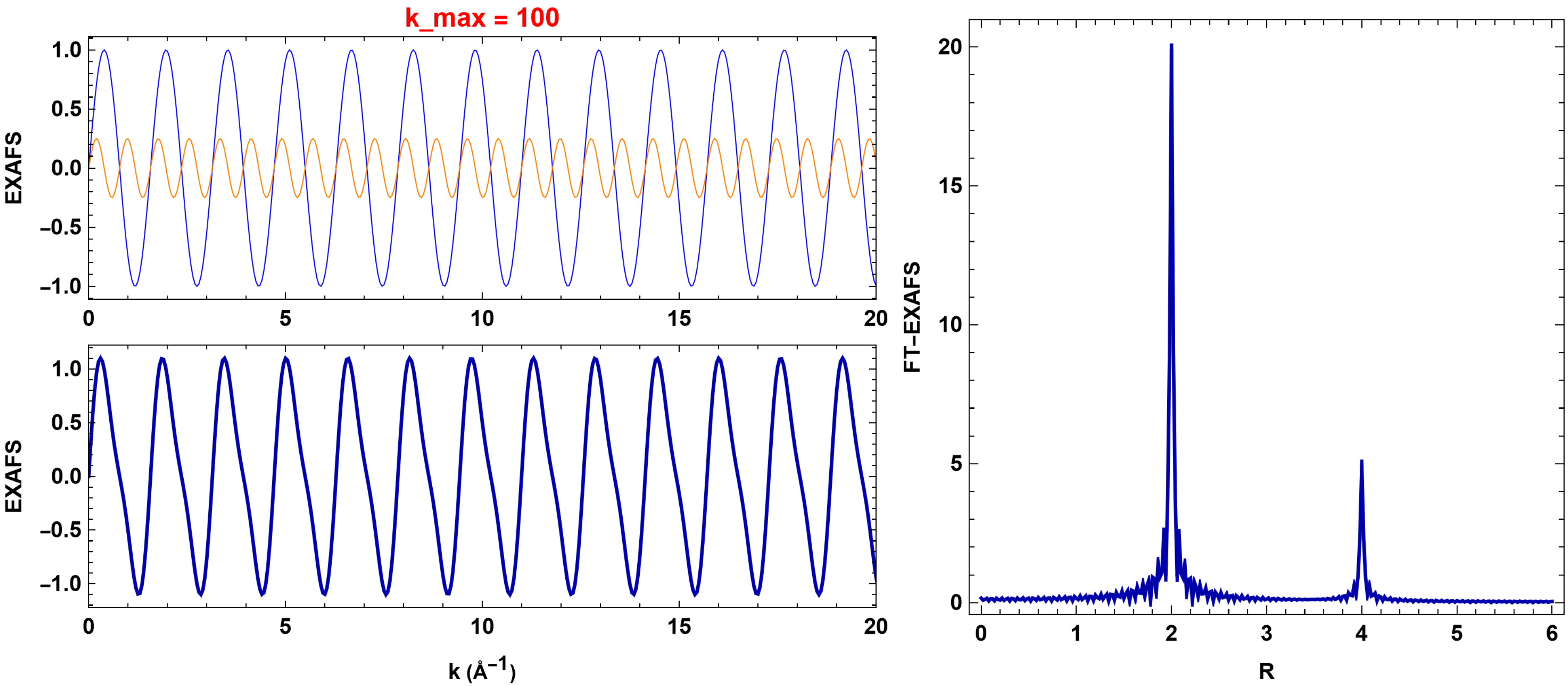

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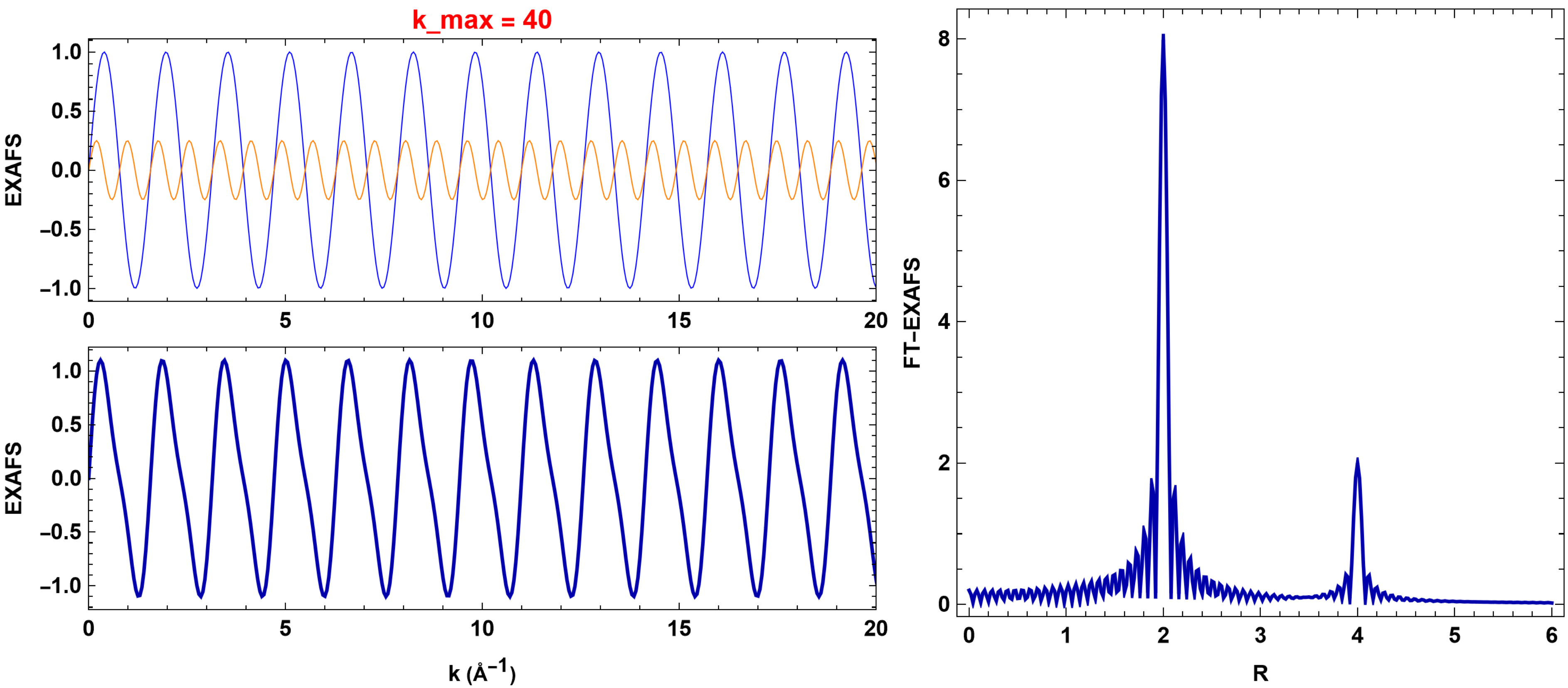

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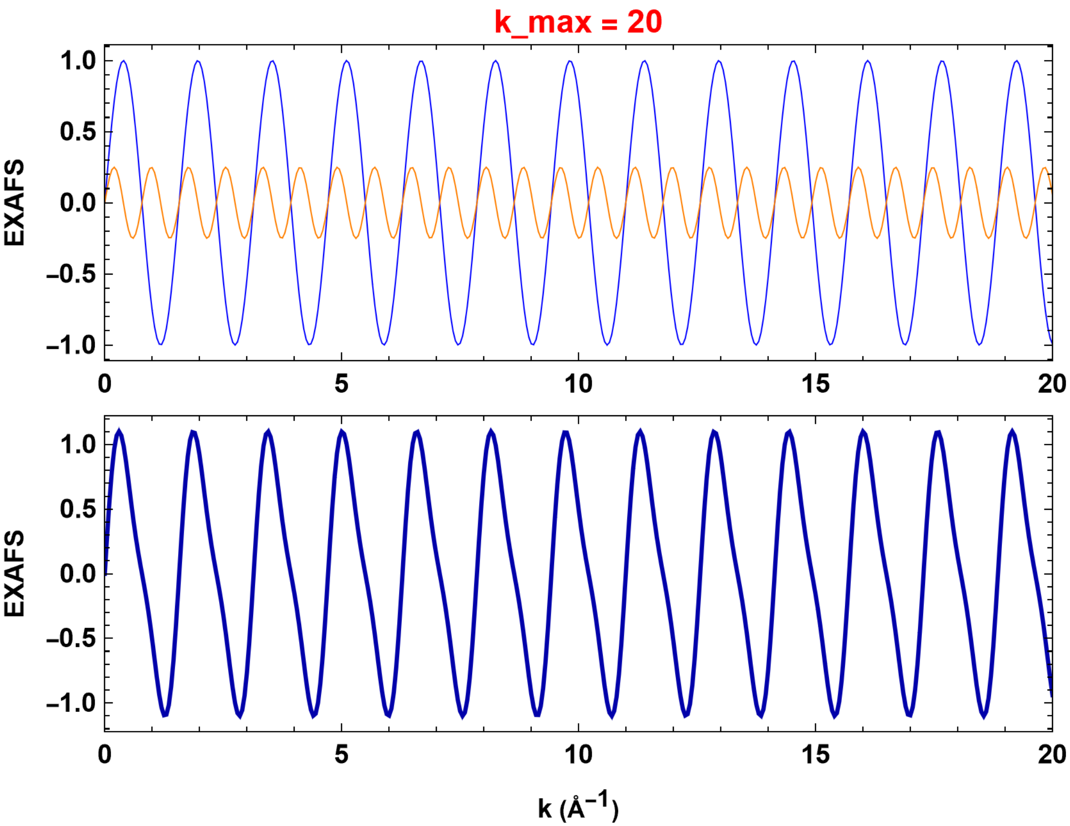

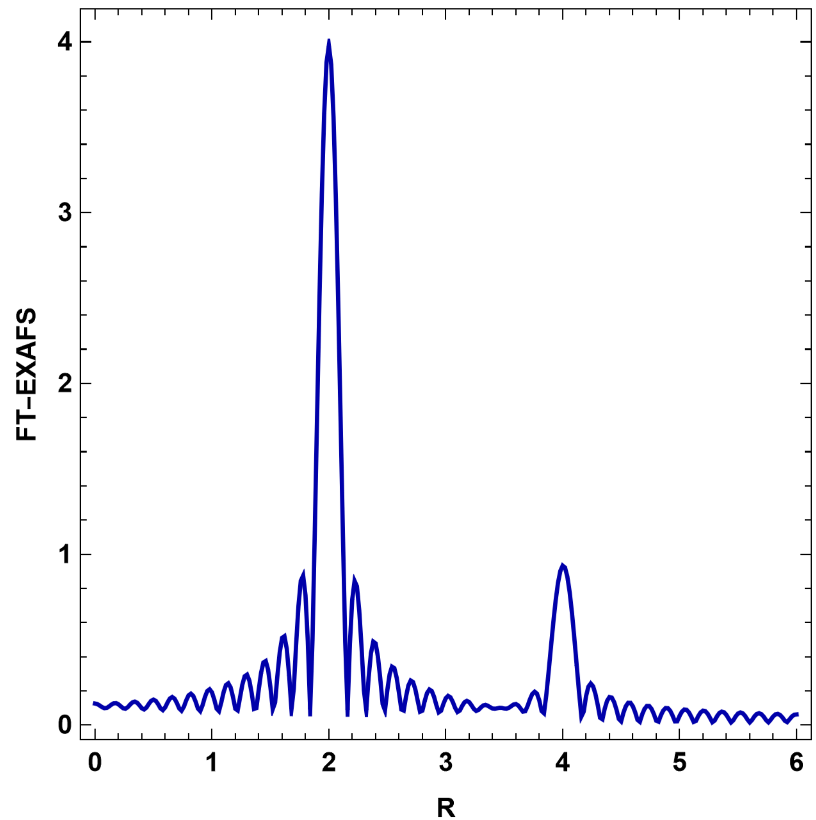

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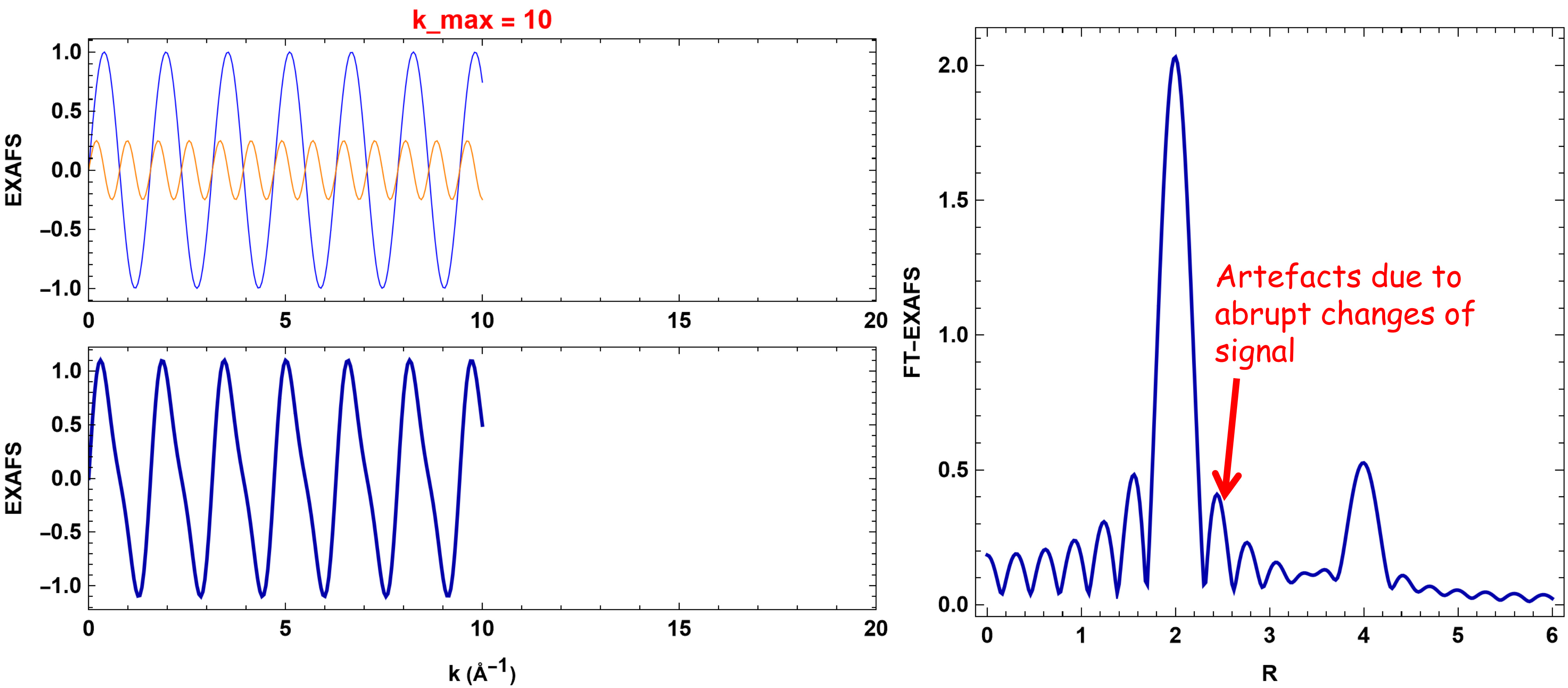
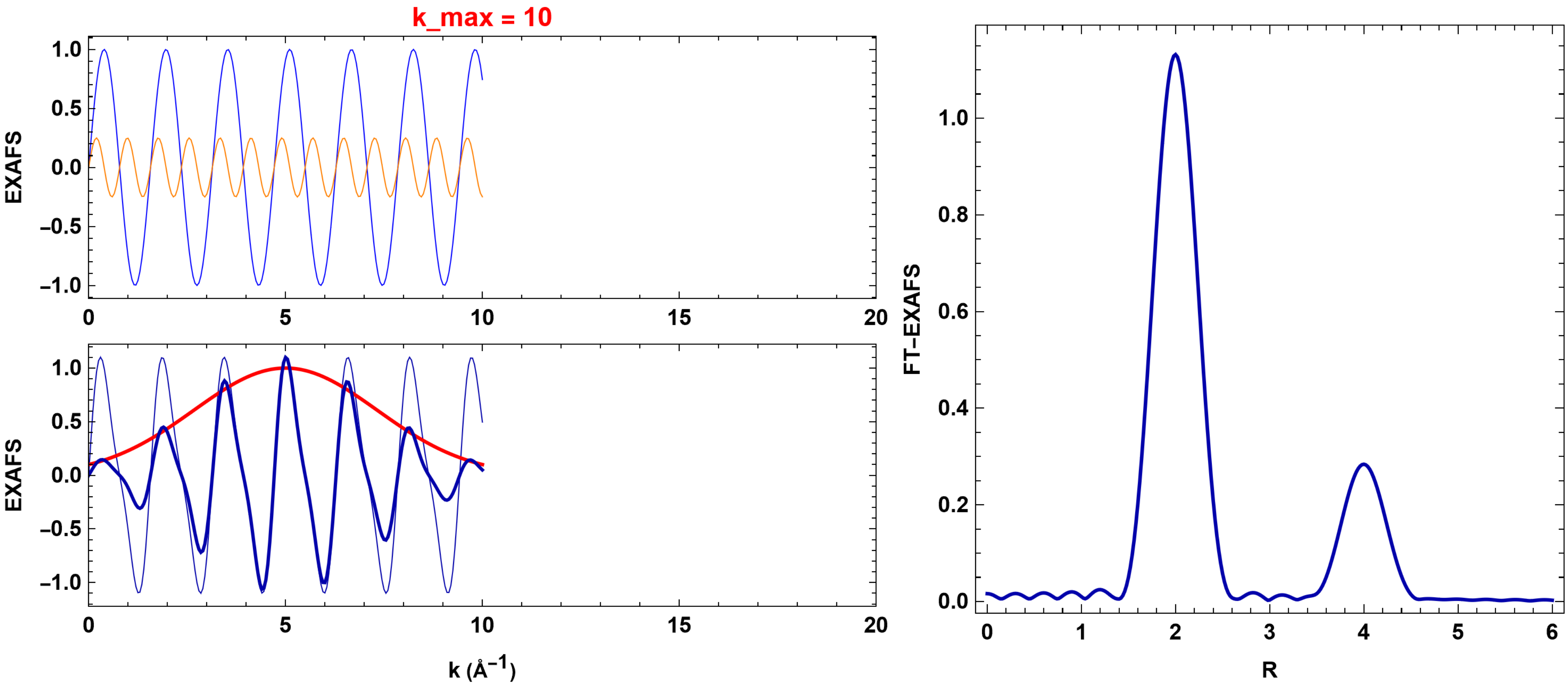


Fourier transform: window function

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p \sin(2kR_p)}{R_p^2}$$

$$FT_\chi(R) = (2\pi)^{-\frac{1}{2}} \int_{k_{min}}^{k_{max}} e^{2iRk} \chi(k) e^{\frac{-(k-k_w)^2}{\sigma_w^2}} dk$$



Fourier transform: disorder factor

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p \sin\left(2kR_p\right) e^{-2k^2\sigma_p^2}}{R_p^2}$$

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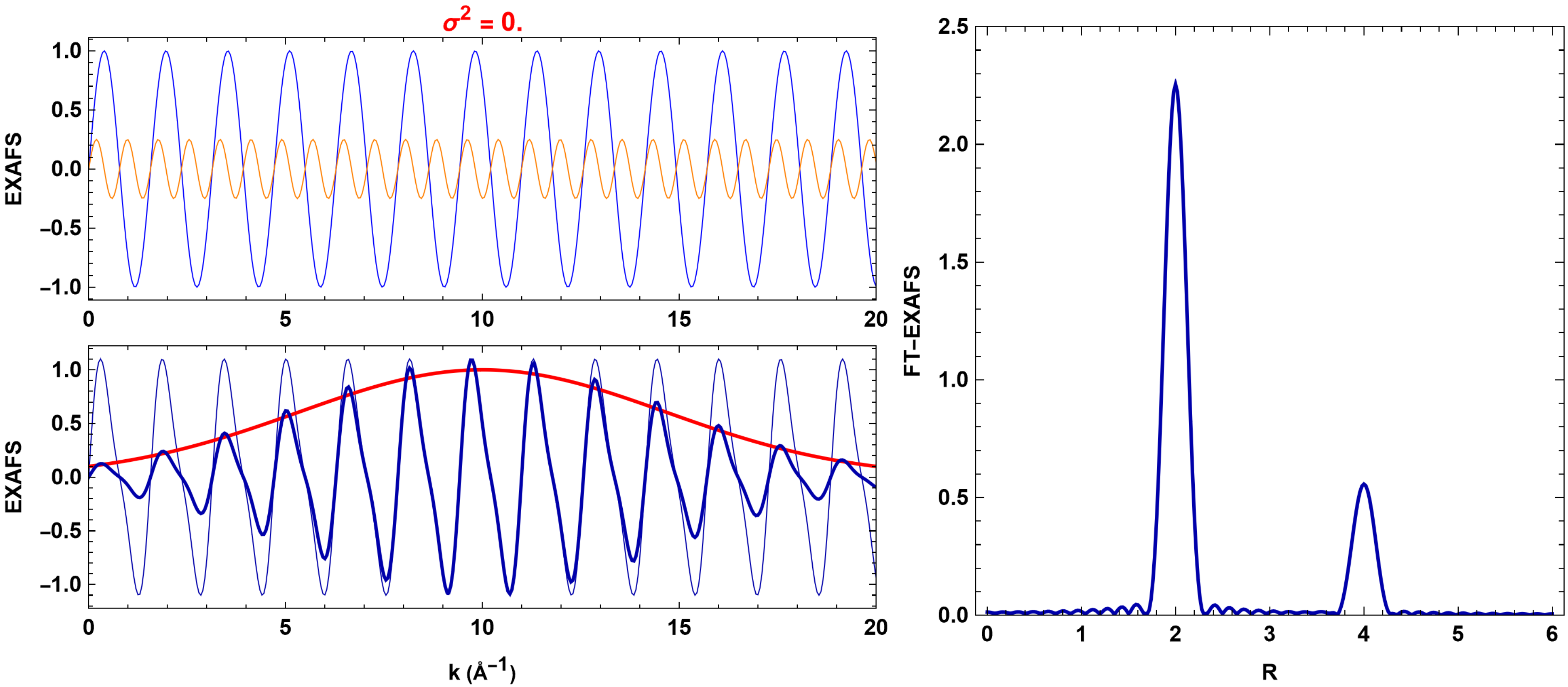

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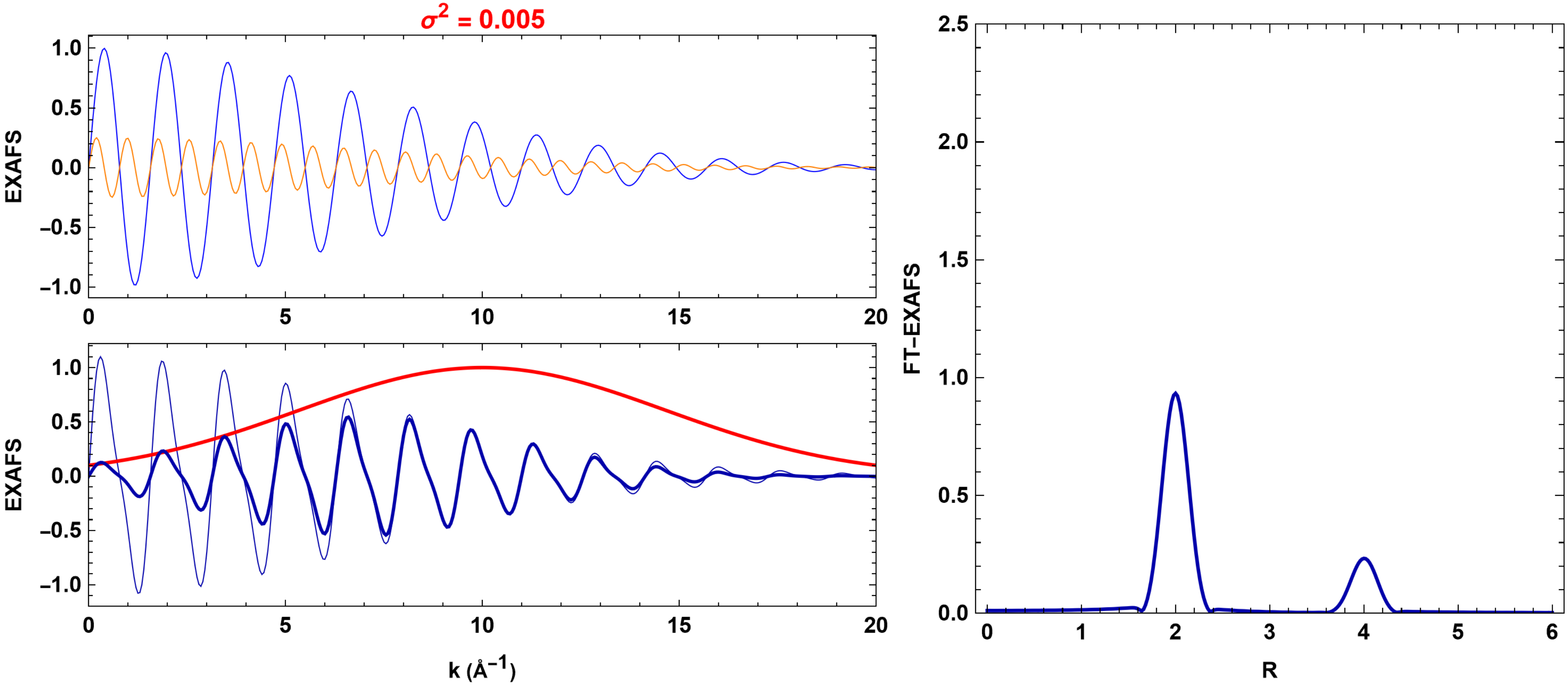

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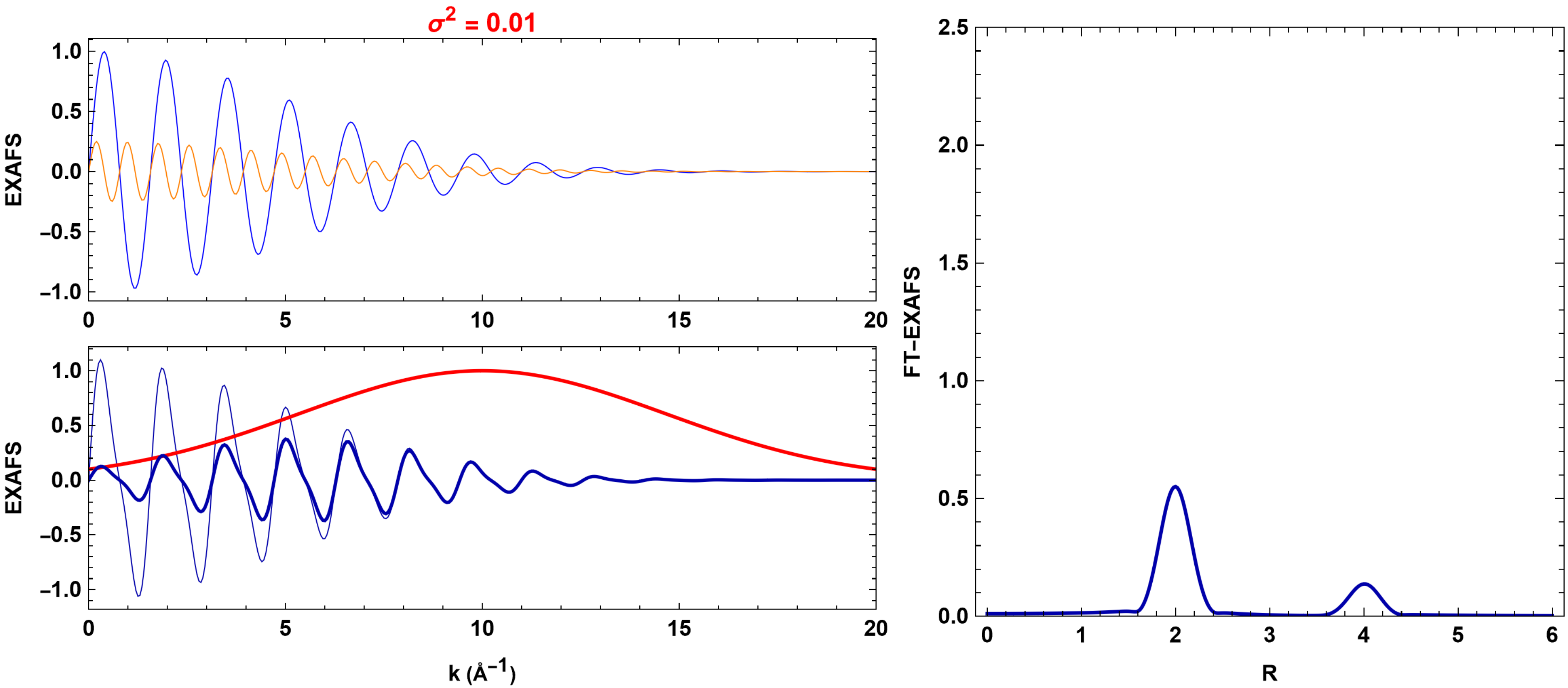
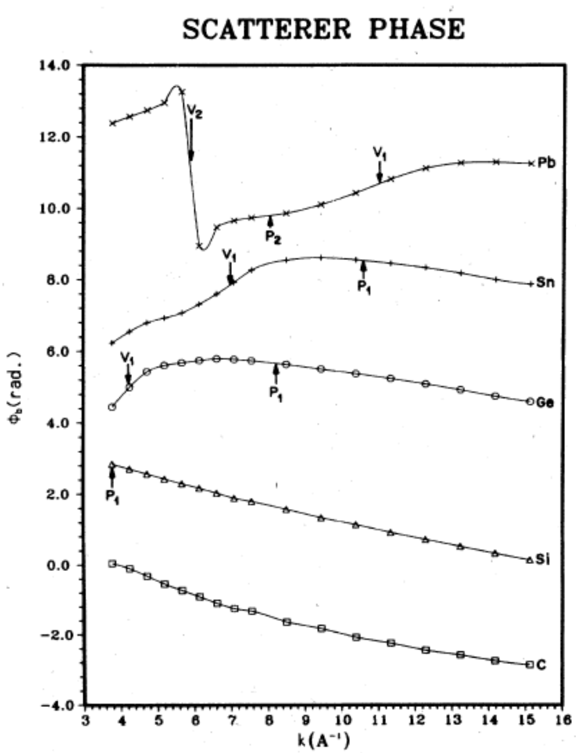


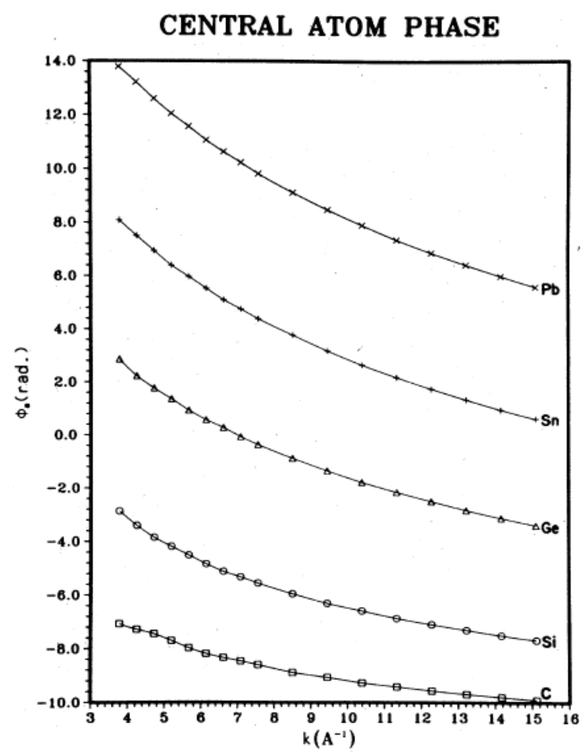
Fourier transform: phase

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p \sin\left(2kR_p + \phi_p(k)\right) e^{-2k^2\sigma_p^2}}{R_p^2}$$

Scattering **phase** $\phi(k) = \phi_{scatterer}(k) + \phi_{central\ atom}(k)$:
different for different types of atoms and result in chemical sensitivity of EXAFS analysis
Phase and amplitude depend on material and can be calculated, e.g., by FEFF

"Real Space Multiple Scattering Calculation of XANES," A.L. Ankudinov, B. Ravel, J.J. Rehr, and S.D. Conradson, Phys. Rev. B 58, 7565 (1998).





P. A. Lee, P. H. Citrin, P. Eisenberger, B. M. Kincaid, Rev. Mod. phys. 53 (1981) 769-806.

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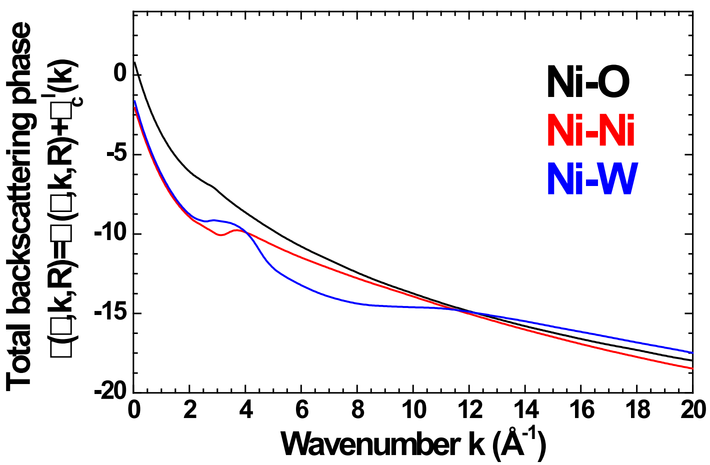

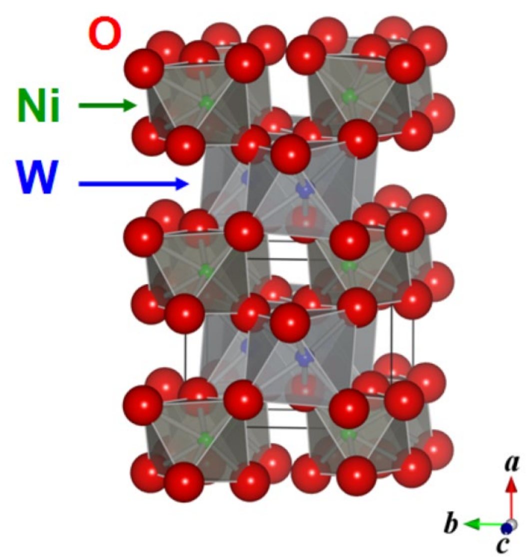

Kuzmin et al, Cent. Eur. J. Phys. • 9(2) • 2011 • 502-509

Fourier transform: phase

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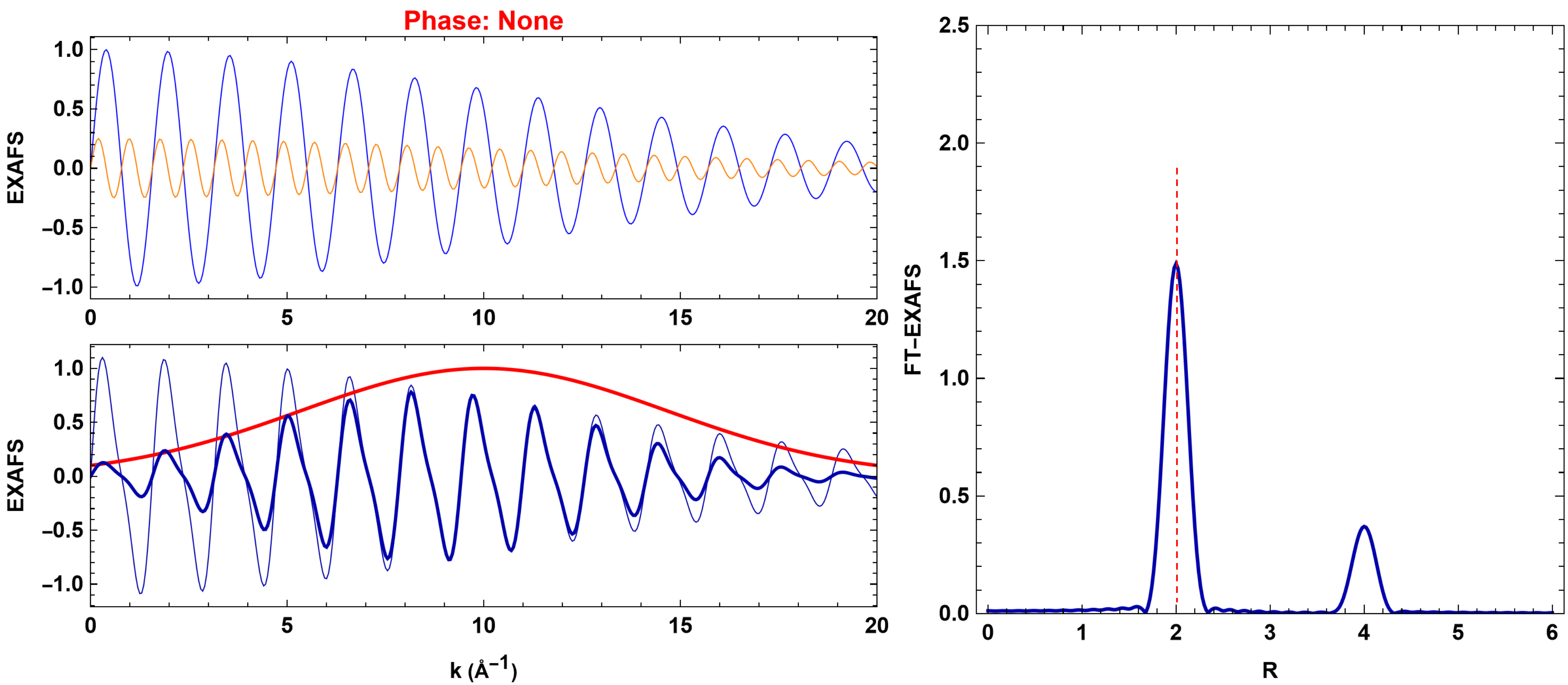

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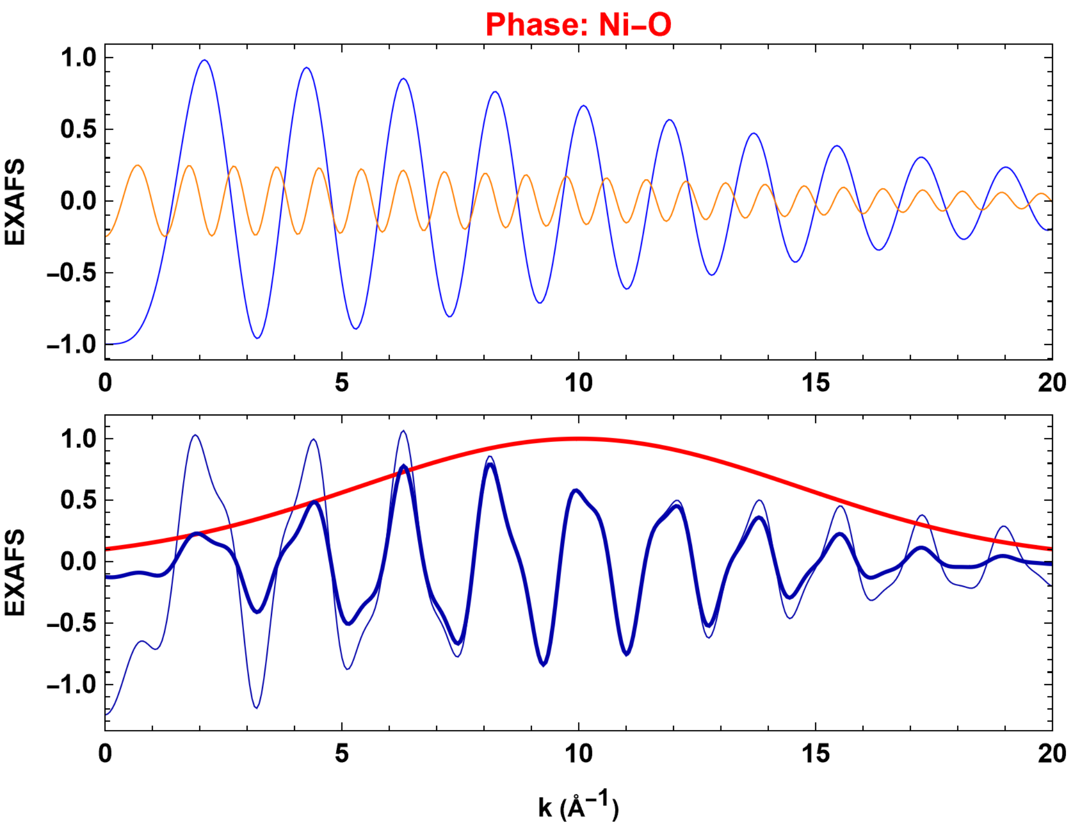

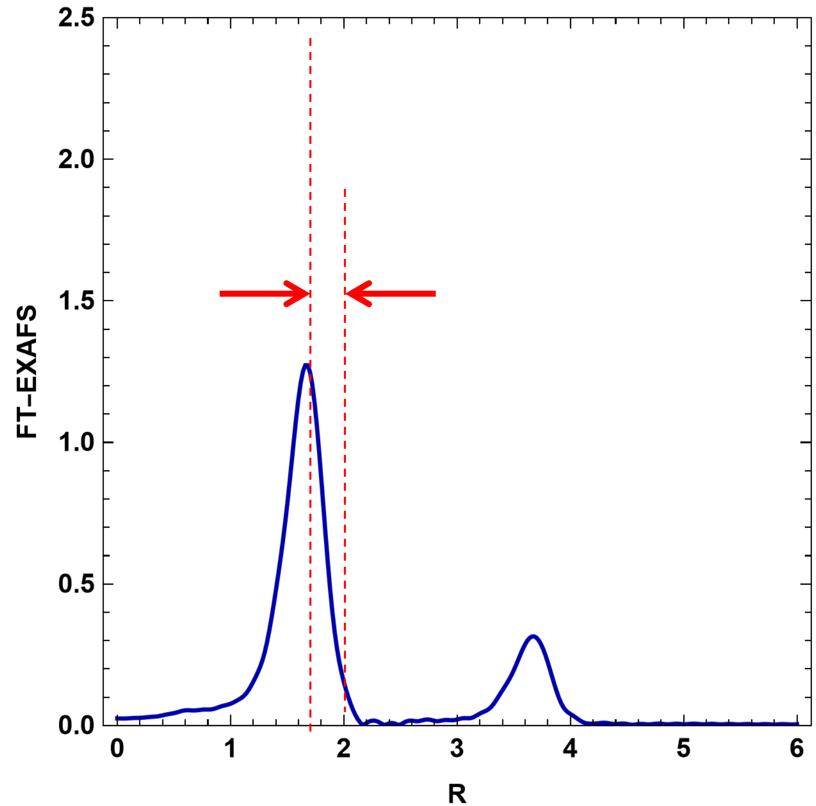

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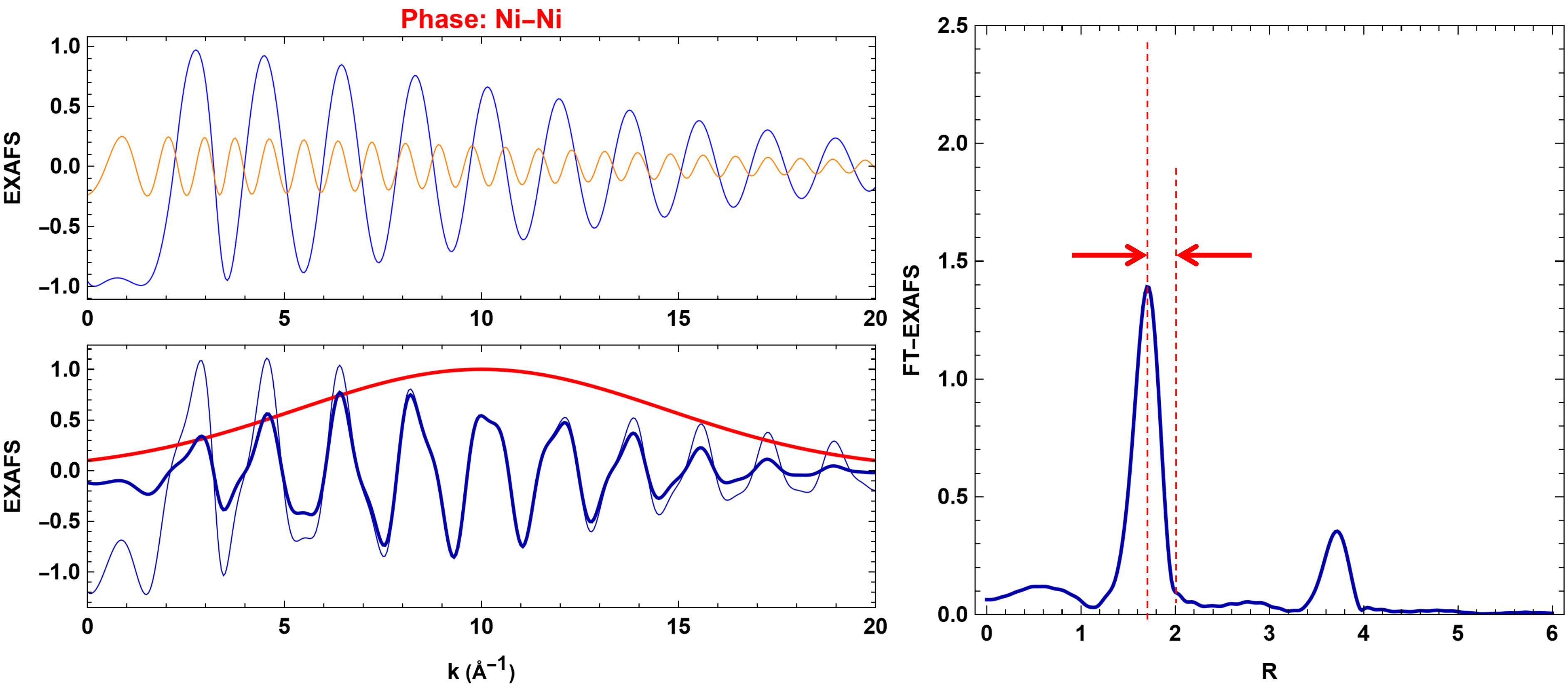

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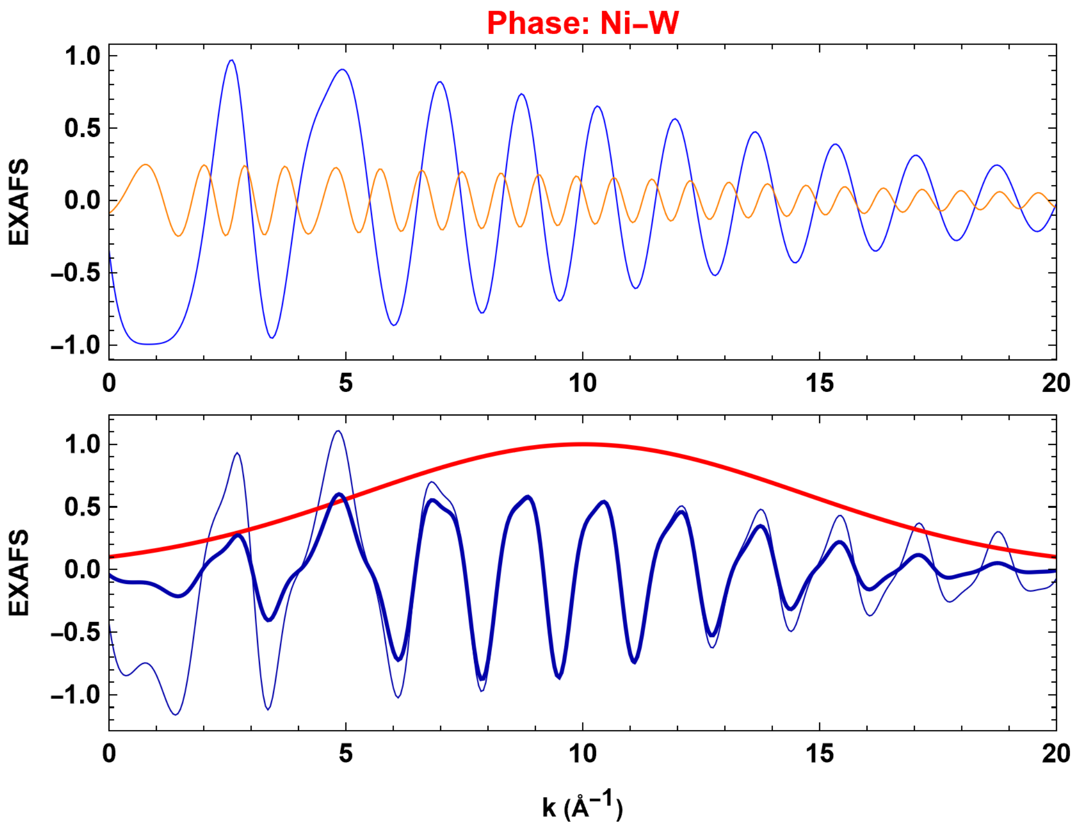
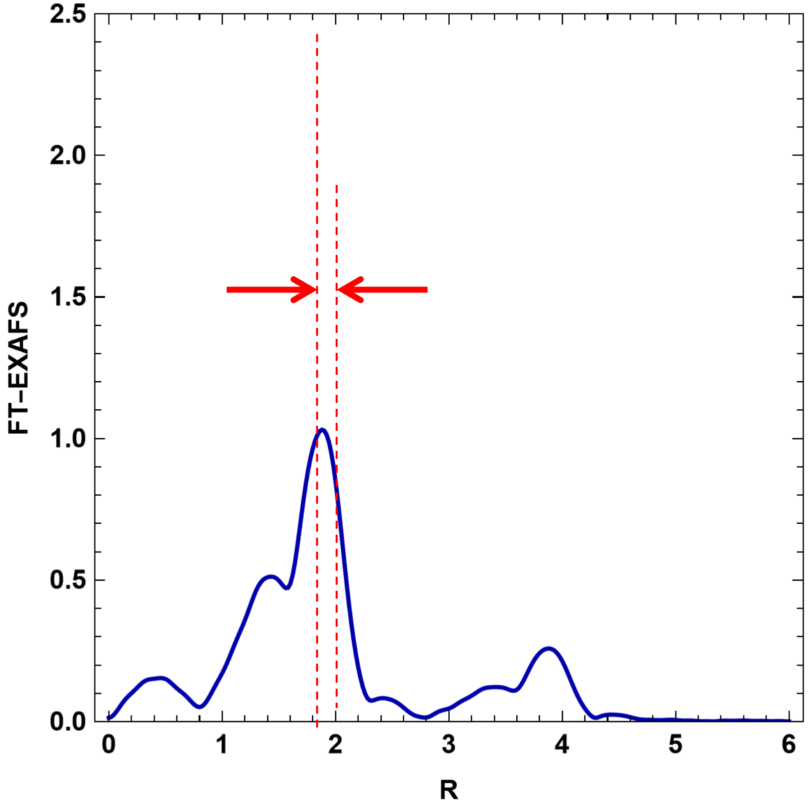
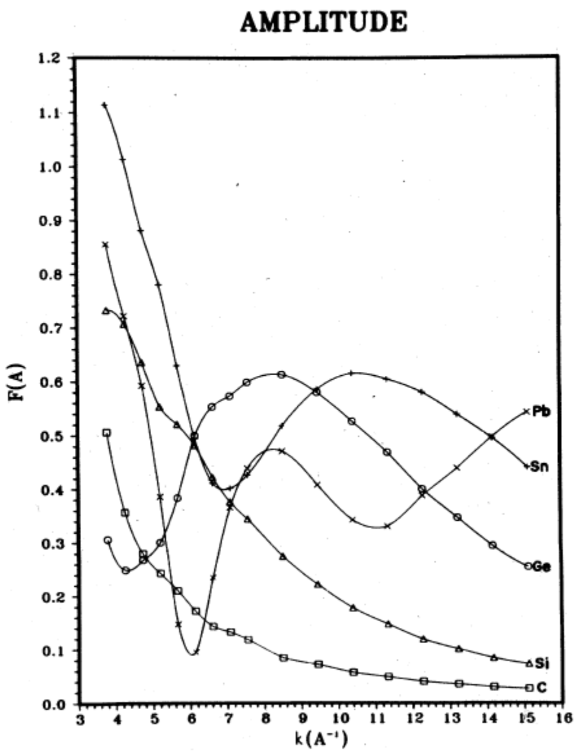
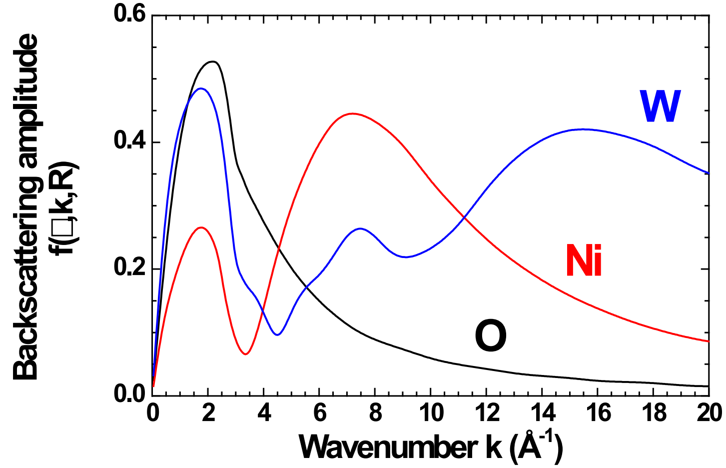


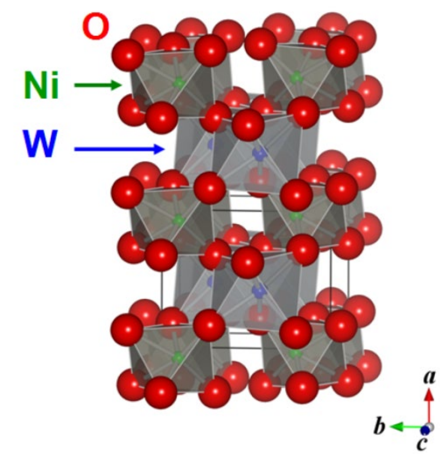


Fourier transform: amplitude

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p f_p(k)\sin\left(2kR_p + \phi_p(k)\right) e^{-2k^2\sigma_p^2}}{kR_p^2}$$







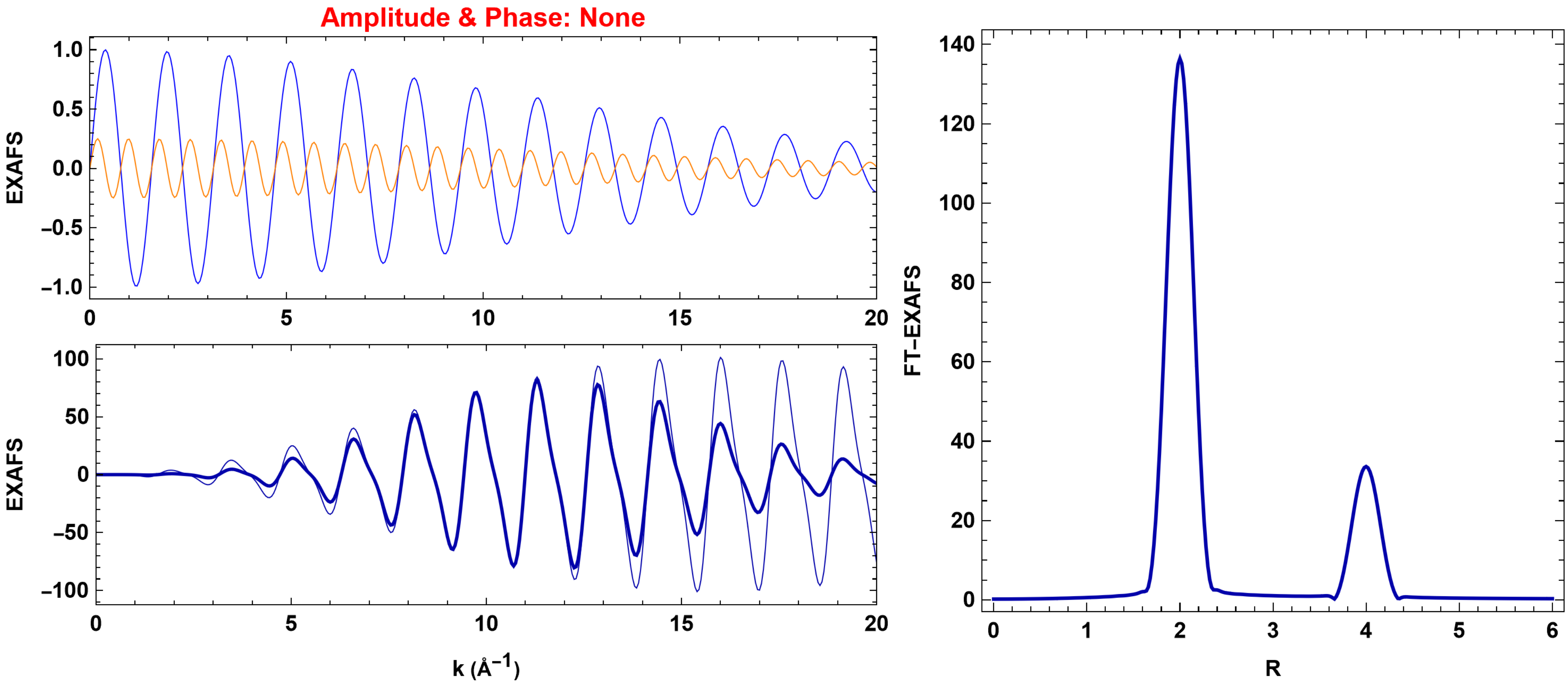
P. A. Lee, P. H. Citrin, P. Eisenberger, B. M. Kincaid, Rev. Mod. phys. 53 (1981) 769-806.

Kuzmin et al, Cent. Eur. J. Phys. • 9(2) • 2011 • 502-509

Fourier transform: amplitude

$$\chi(k) = \sum_p S_0^2 N_p \frac{f_p(k)}{kR_p^2} e^{-2k^2\sigma_p^2} \sin\left(2kR_p + \phi_p(k)\right) \rightarrow \sum_p \frac{S_0^2 N_p f_p(k) \sin\left(2kR_p + \phi_p(k)\right) e^{-2k^2\sigma_p^2}}{kR_p^2}$$

$$FT_\chi(R) = (2\pi)^{-\frac{1}{2}} \int_{k_{min}}^{k_{max}} e^{2iRk} \chi(k) k^2 e^{\frac{-(k-k_w)^2}{\sigma_w^2}} dk$$



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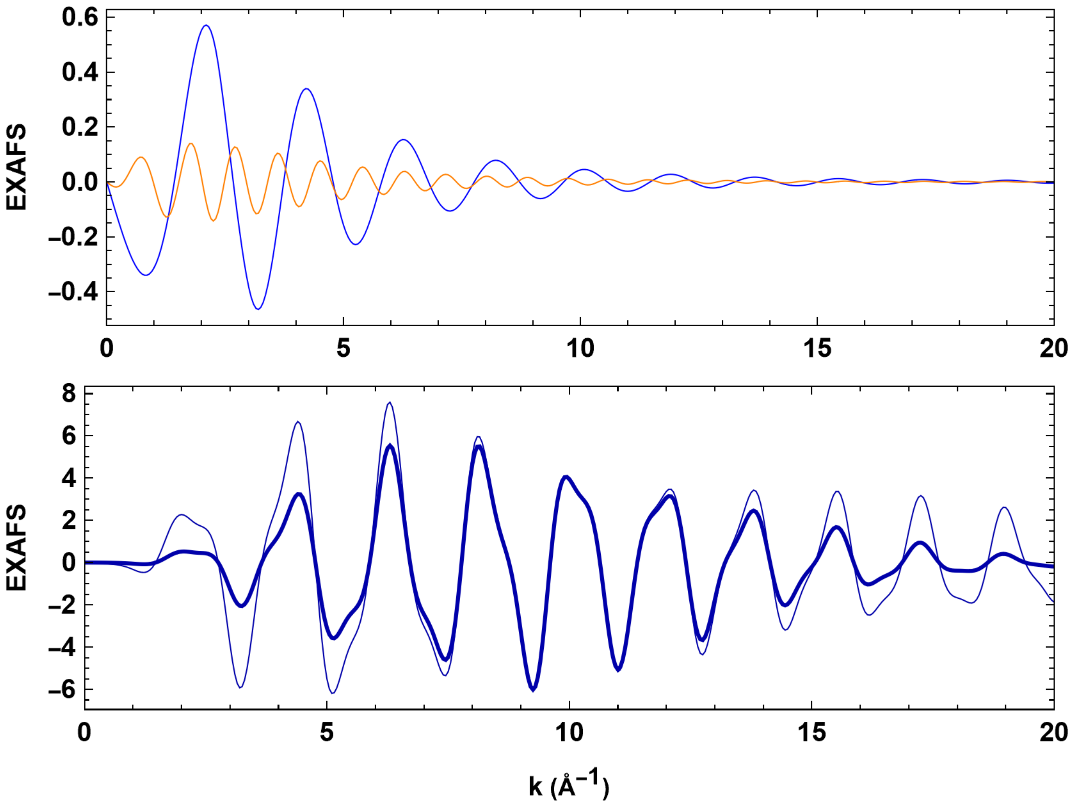
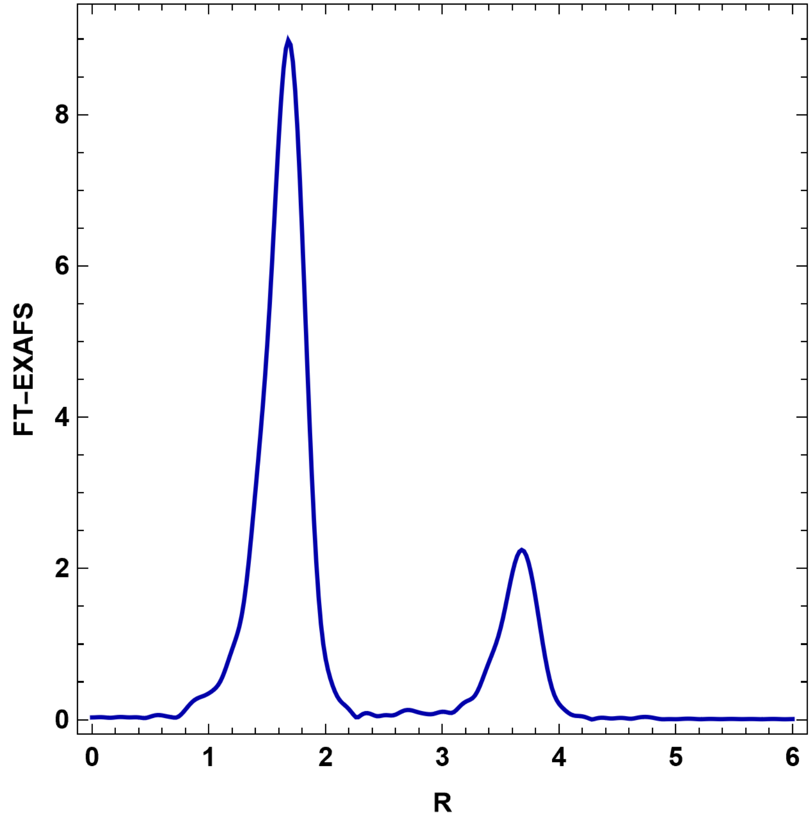
Amplitude & Phase: Ni–O





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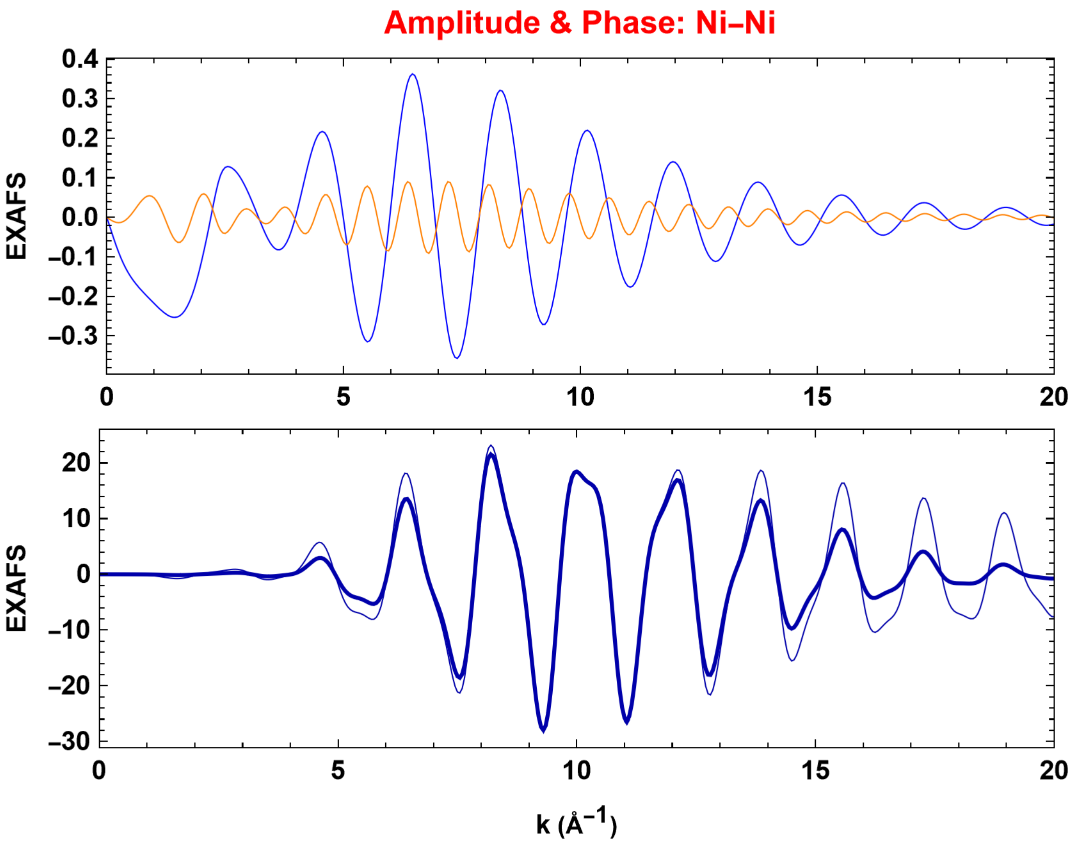

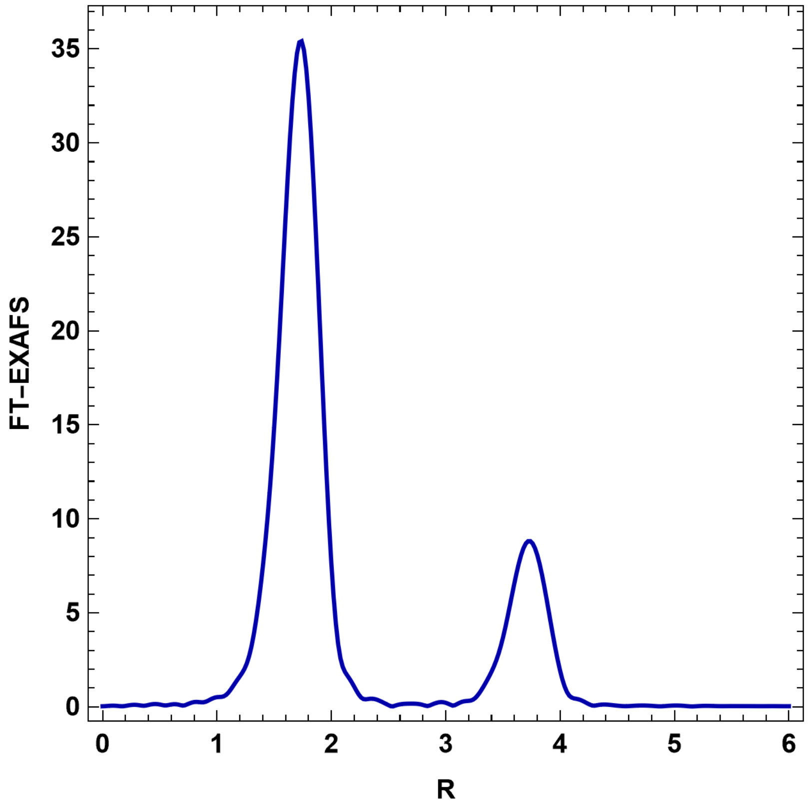

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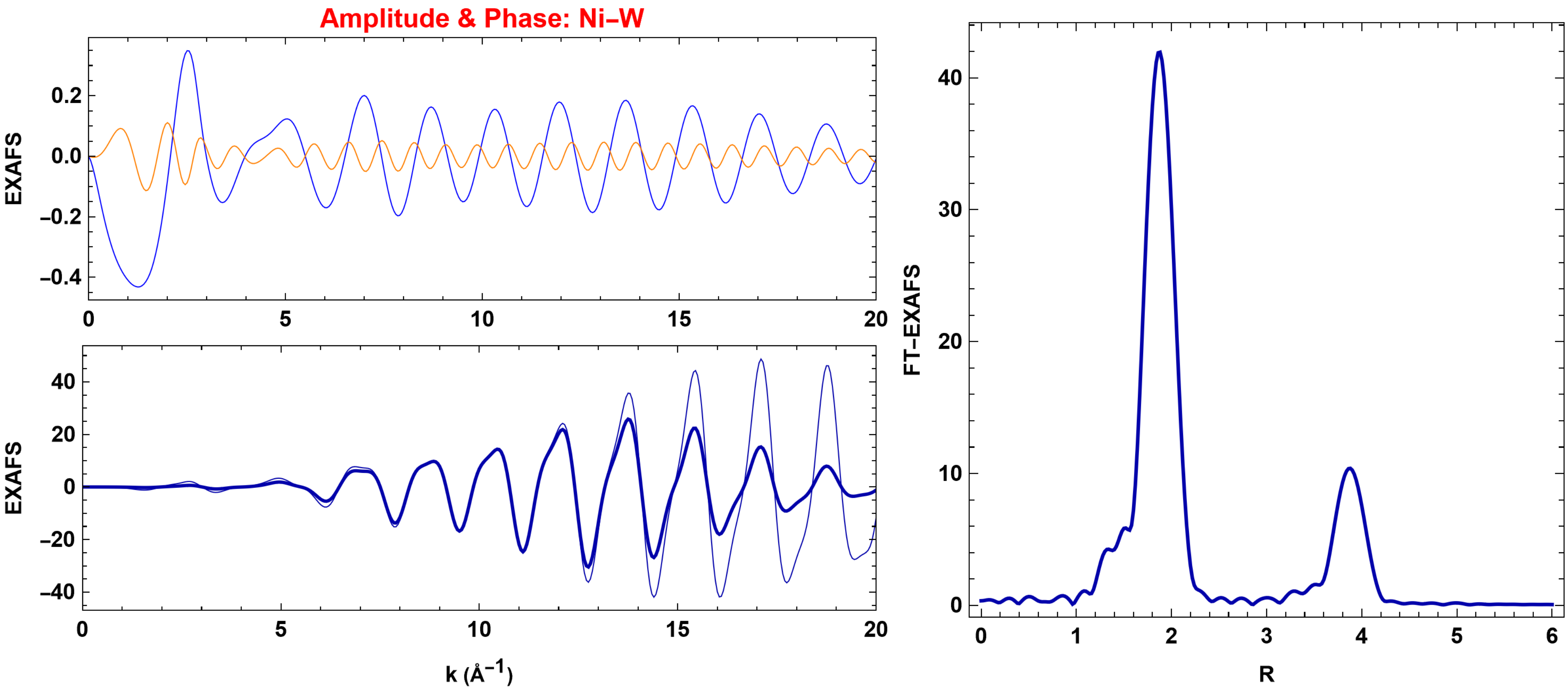

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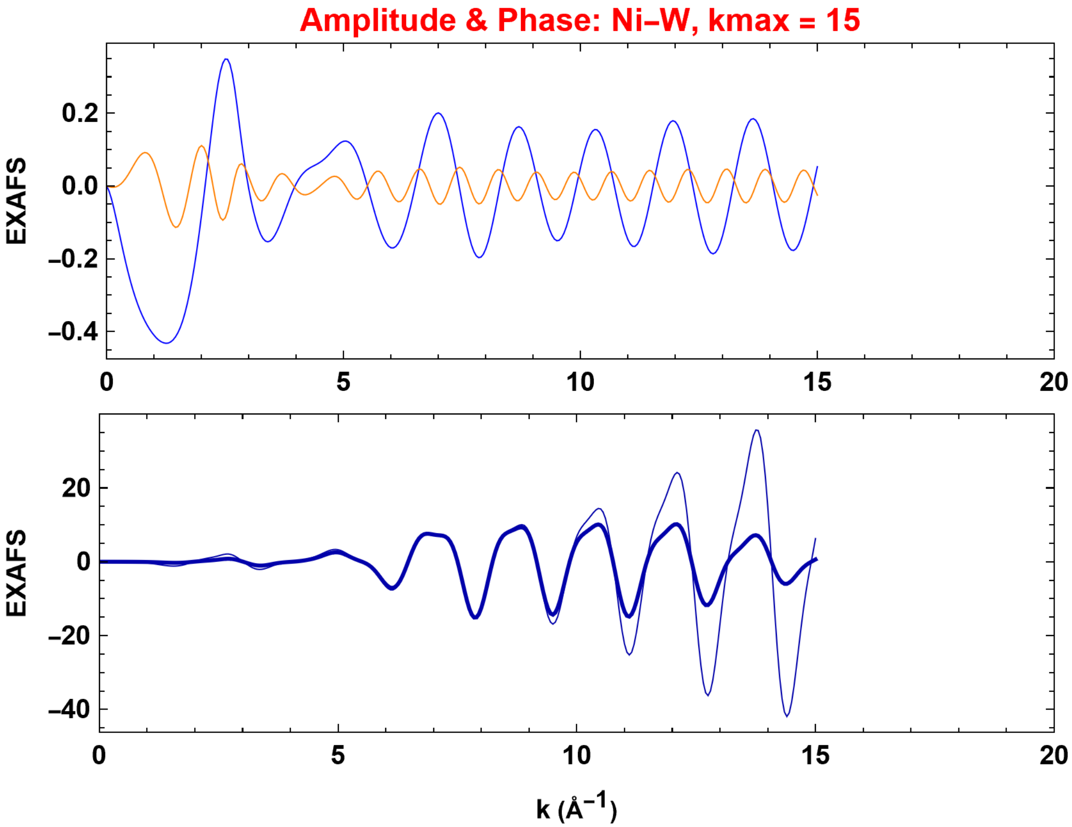
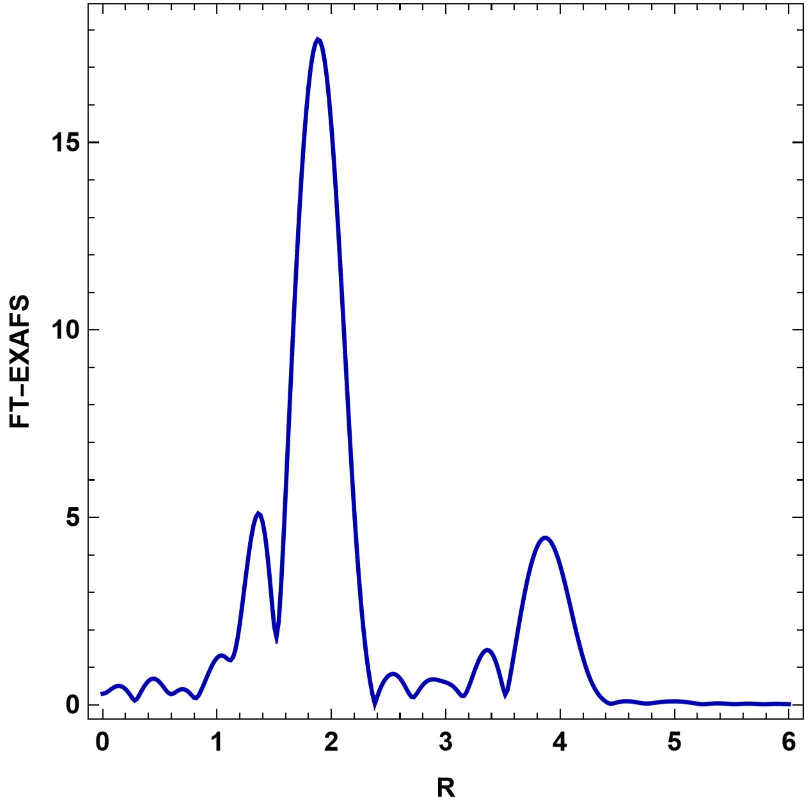




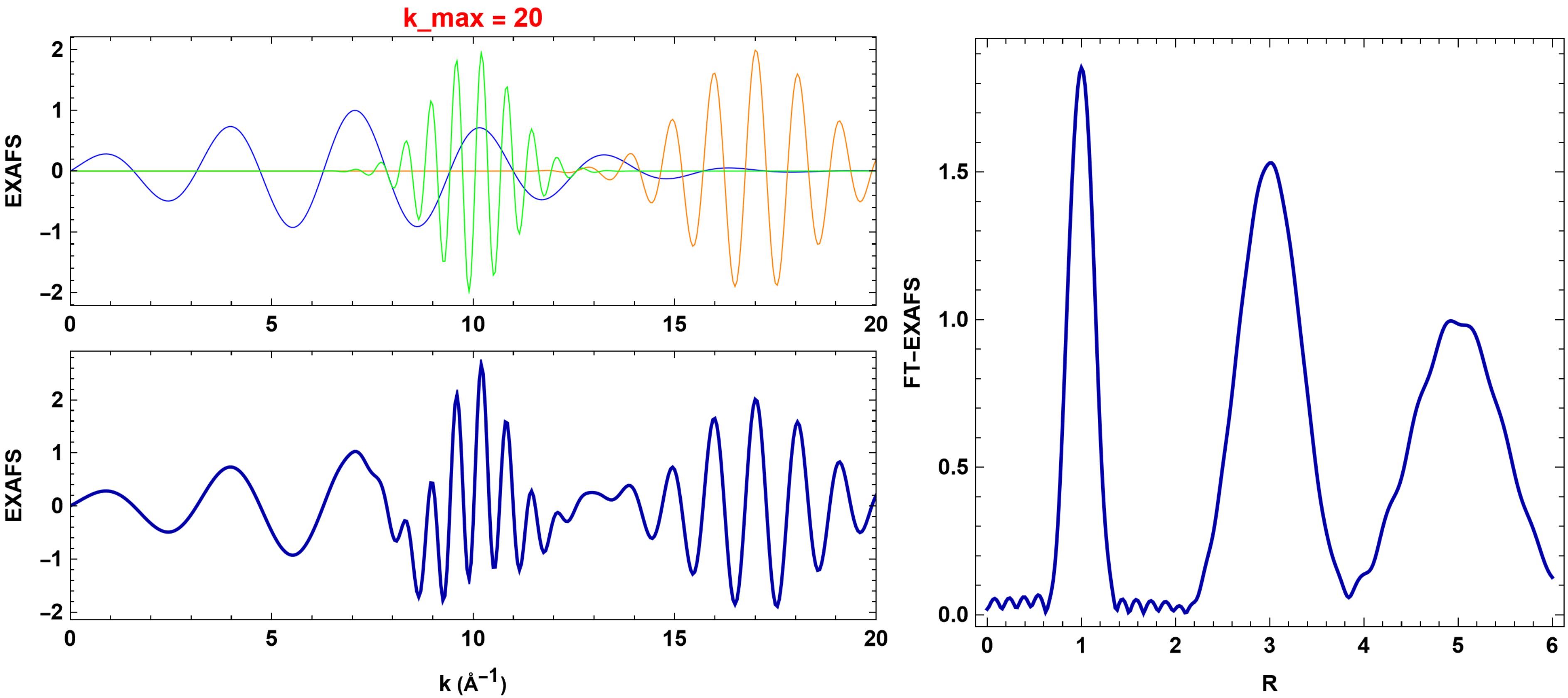
FT-EXAFS: summary

- There are many structure-unrelated factors that can affect number, position and shape of FT peaks
- Chemical sensitivity of FT-EXAFS is very limited: e.g., Ni-O and Ni-Ni peaks in FT-EXAFS look very similar, since information about location of spectral components in *k*-space is lost

Short-time Fourier transform

$$\chi(k) = \sum_p N_p e^{-2(k-k_0)^2\sigma_p^2} \sin(2kR_p)$$

$$FT_\chi(R) = (2\pi)^{-\frac{1}{2}} \int_{k_{min}}^{k_{max}} e^{2iRk} \chi(k) k^2 e^{\frac{-(k-k_w)^2}{\sigma_w^2}} dk$$



No information in FT-EXAFS about location of spectral components in k-space

Short-time Fourier transform

$$\chi(k) = \sum_p N_p e^{-2(k-k_0)^2 \sigma_p^2} \sin(2kR_p)$$

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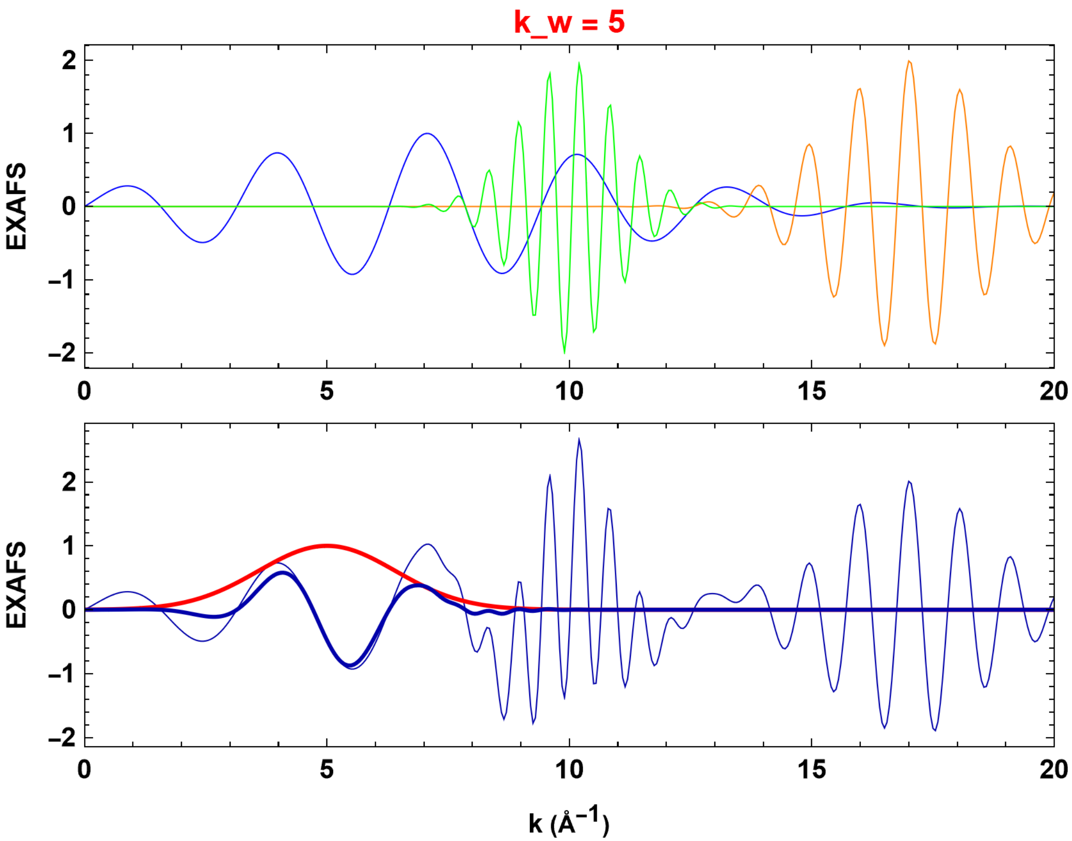

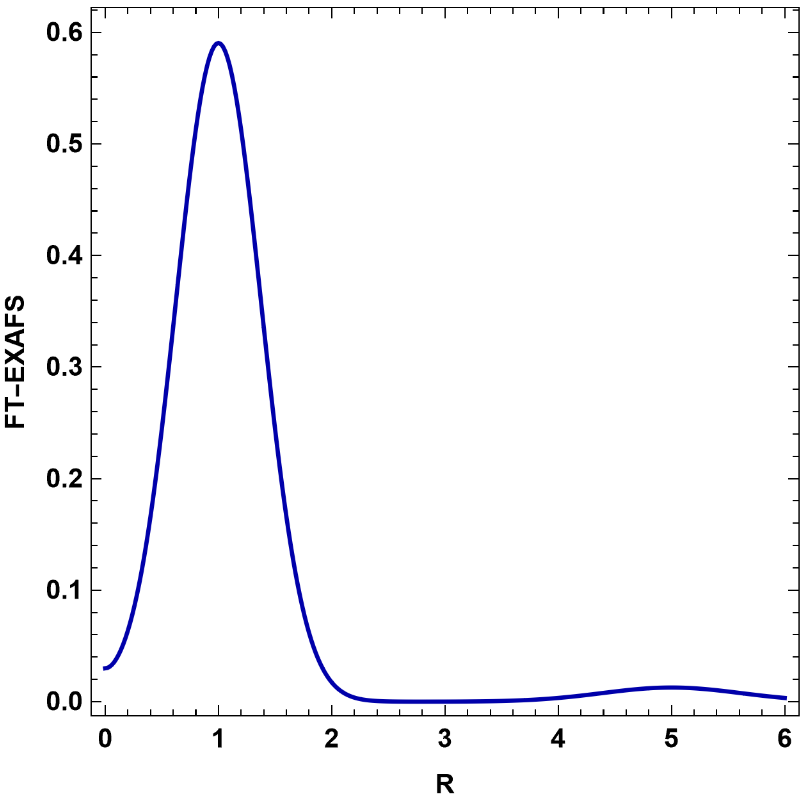

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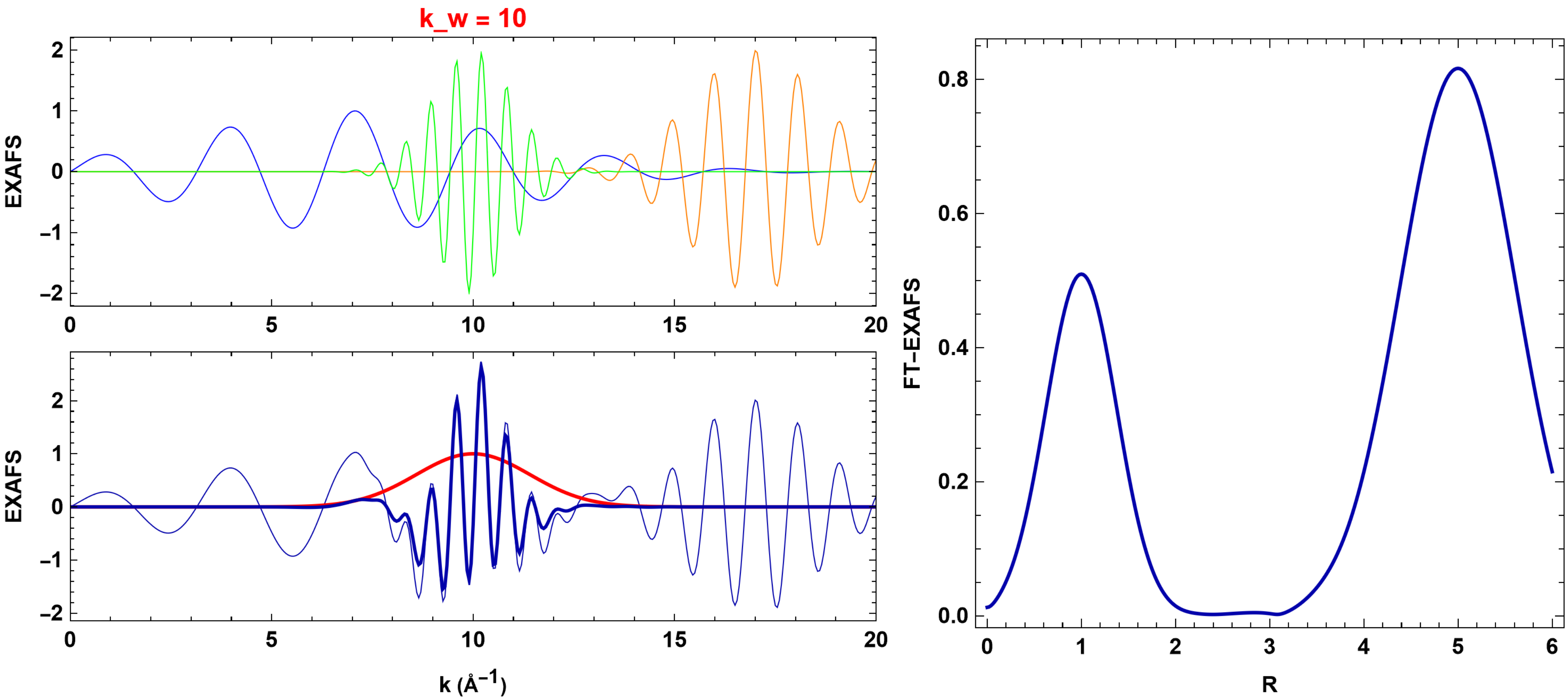

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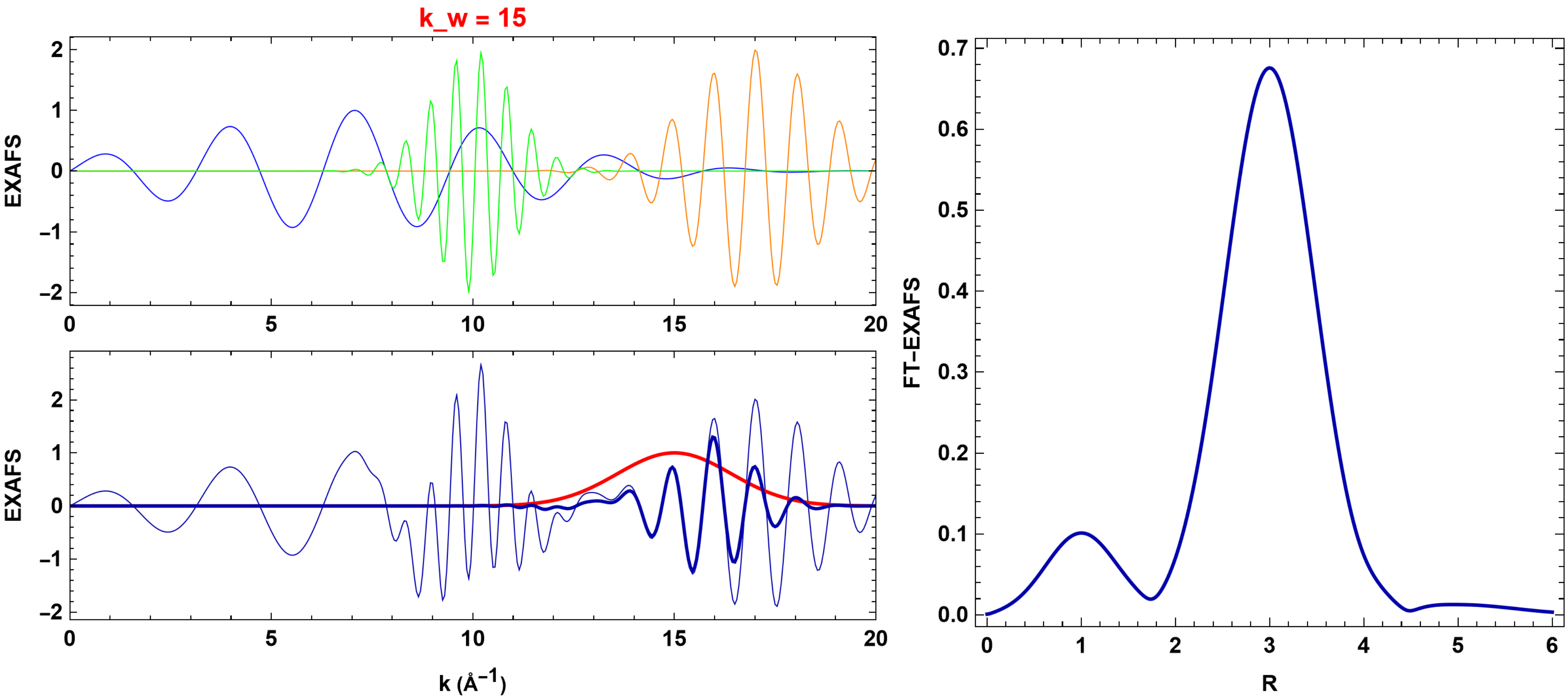

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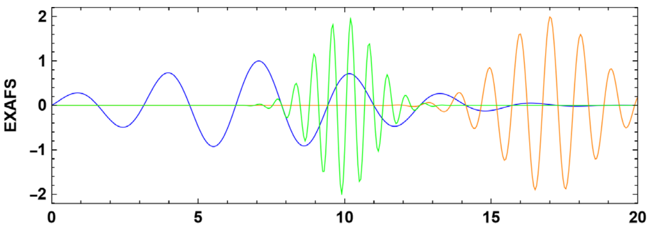

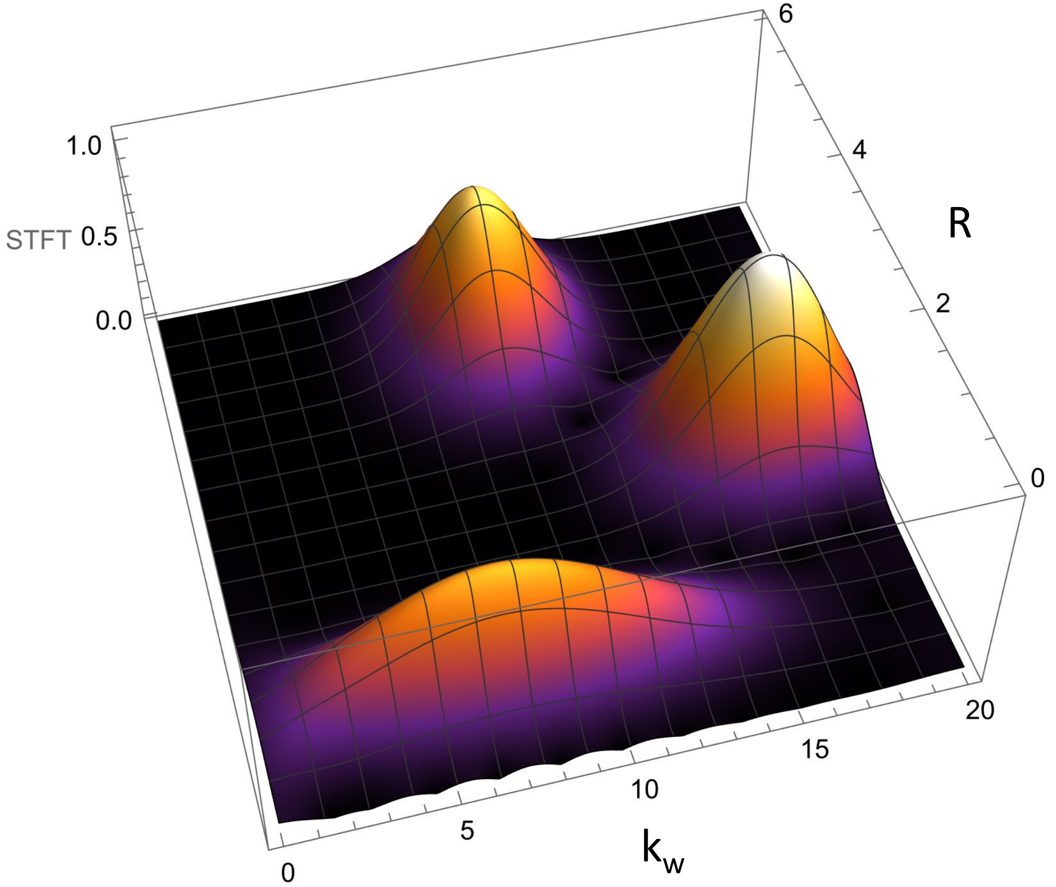

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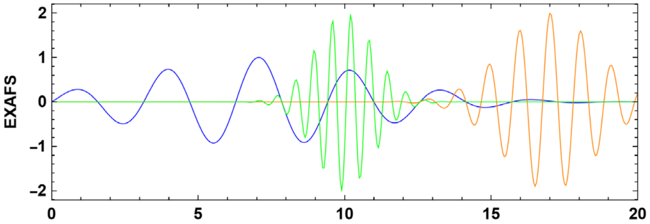

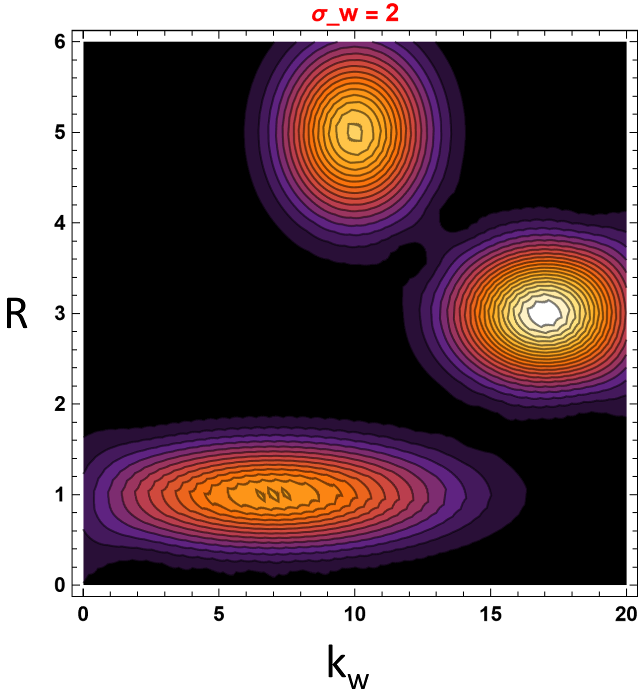

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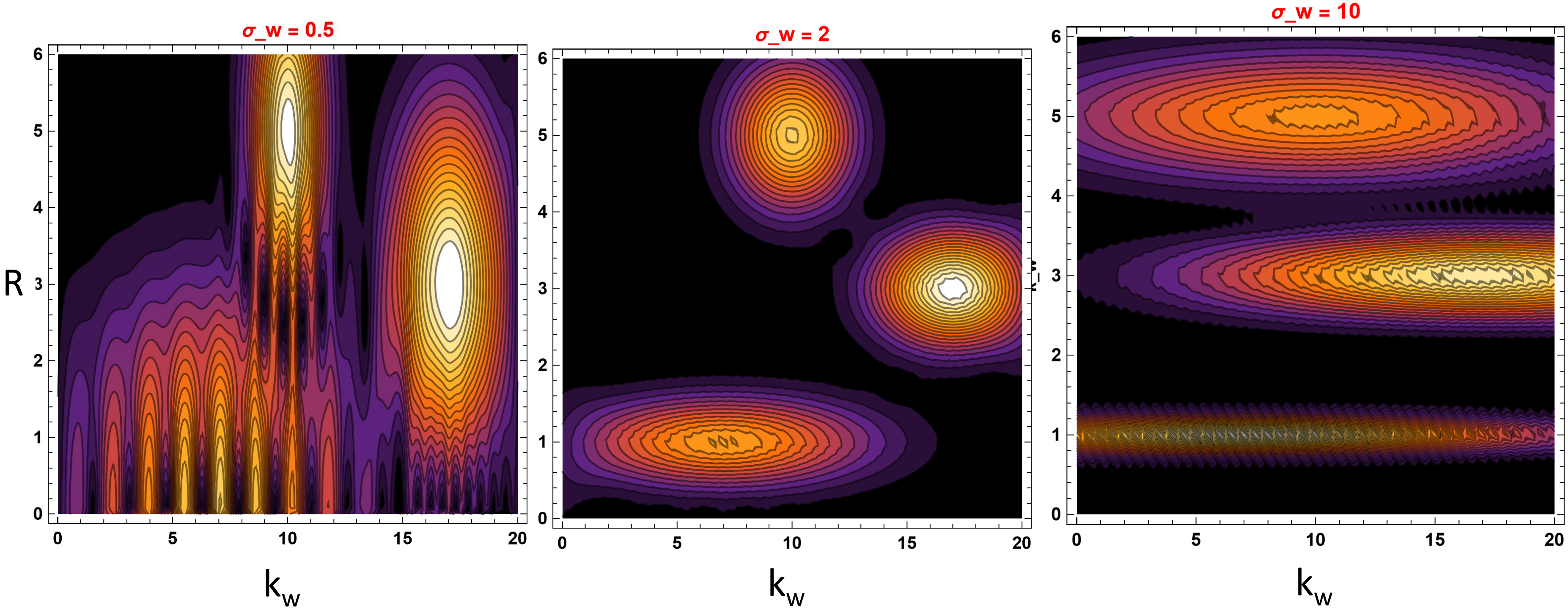


Result depends on the width of window function.
What is the optimal width? – it depends on frequency

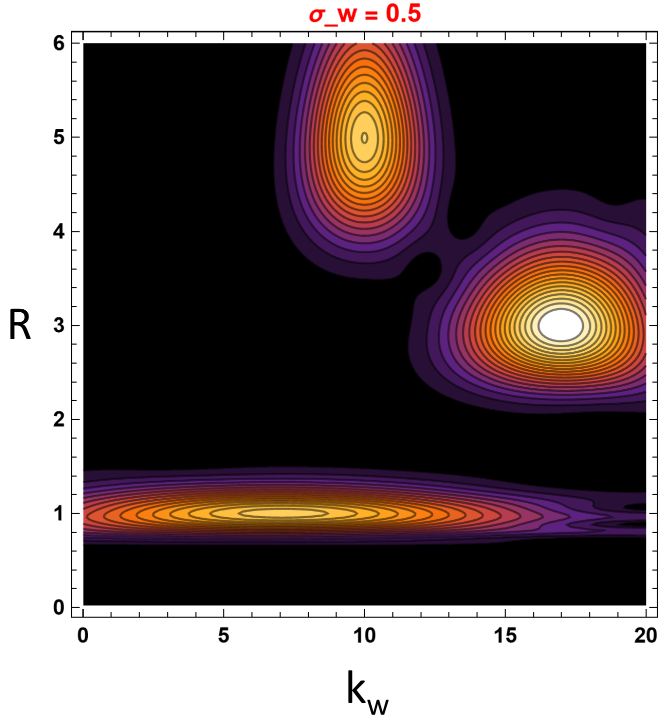
Morlet wavelet transform

$$\chi(k) = \sum_p N_p e^{-2(k-k_0)^2\sigma_p^2} \sin(2kR_p)$$

$$WT_\chi(k,R) = (R/R_0)^{\frac{1}{2}} \int_{k_{min}}^{k_{max}} e^{-2iR(k'-k)} \chi(k') k'^2 e^{\frac{-(k'-k)^2}{(R_0/R)^2\,\sigma_0^2}} dk'$$

$$= (R/R_0)^{\frac{1}{2}} \int_{k_{min}}^{k_{max}} \phi\left(\frac{k'-k}{R_0/R}\right) \chi(k') k'^2 dk', \text{ where}$$

$$\phi(k) = \exp(-2iR_0k)\exp(-k^2/\sigma_0^2)$$

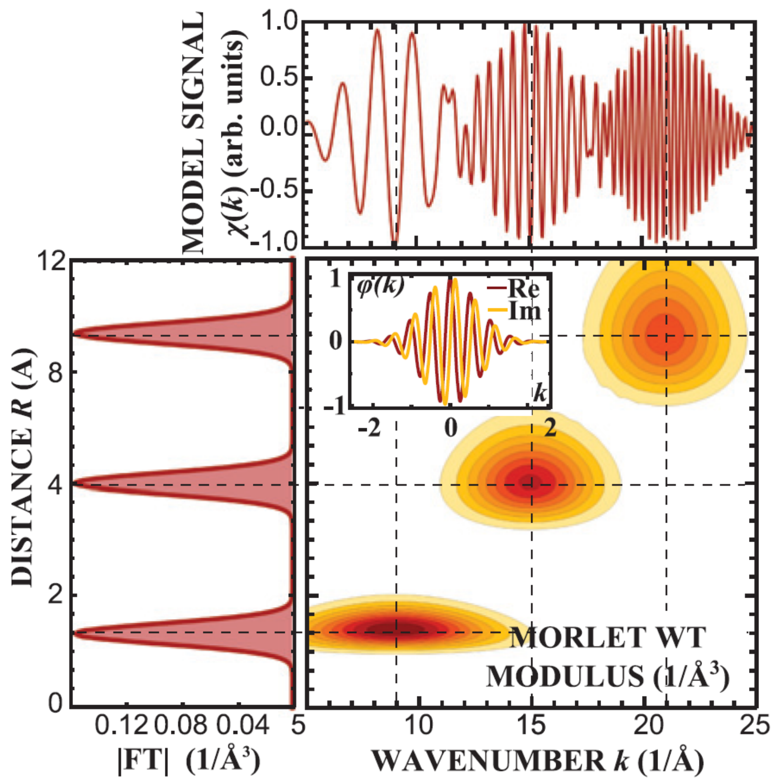


Window function width $\sim\sigma_0^2 R_0/R$ – different for different frequencies!

Morlet wavelet transform

$$\chi(k) = \sum_p N_p e^{-2(k-k_0)^2\sigma_p^2} \sin(2kR_p)$$

$$WT_\chi(k,R) = (R/R_0)^{\frac{1}{2}} \int_{k_{min}}^{k_{max}} \phi\left(\frac{k'-k}{R_0/R}\right)\chi(k')k'^2 dk'$$



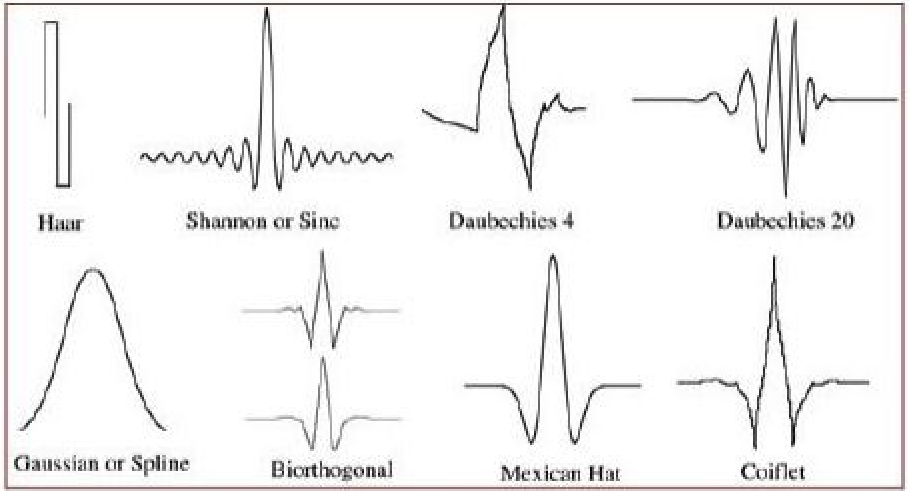
Timoshenko et al,
Z. Phys. Chem. 2016; 230(4): 551–568

Resolution different for different frequencies!

More about wavelet transform

$$WT_\chi(k,R) = (R/R_0)^{\frac{1}{2}} \int_{k_{min}}^{k_{max}} \phi\left(\frac{k'-k}{R_0/R}\right) \chi(k') k'^2 dk'$$

- Some other popular choices for mother wavelet function:



https://georgemdallas.wordpress.com/2014/05/14/wavelets-4-dummies-signal-processing-fourier-transforms-and-heisenberg/

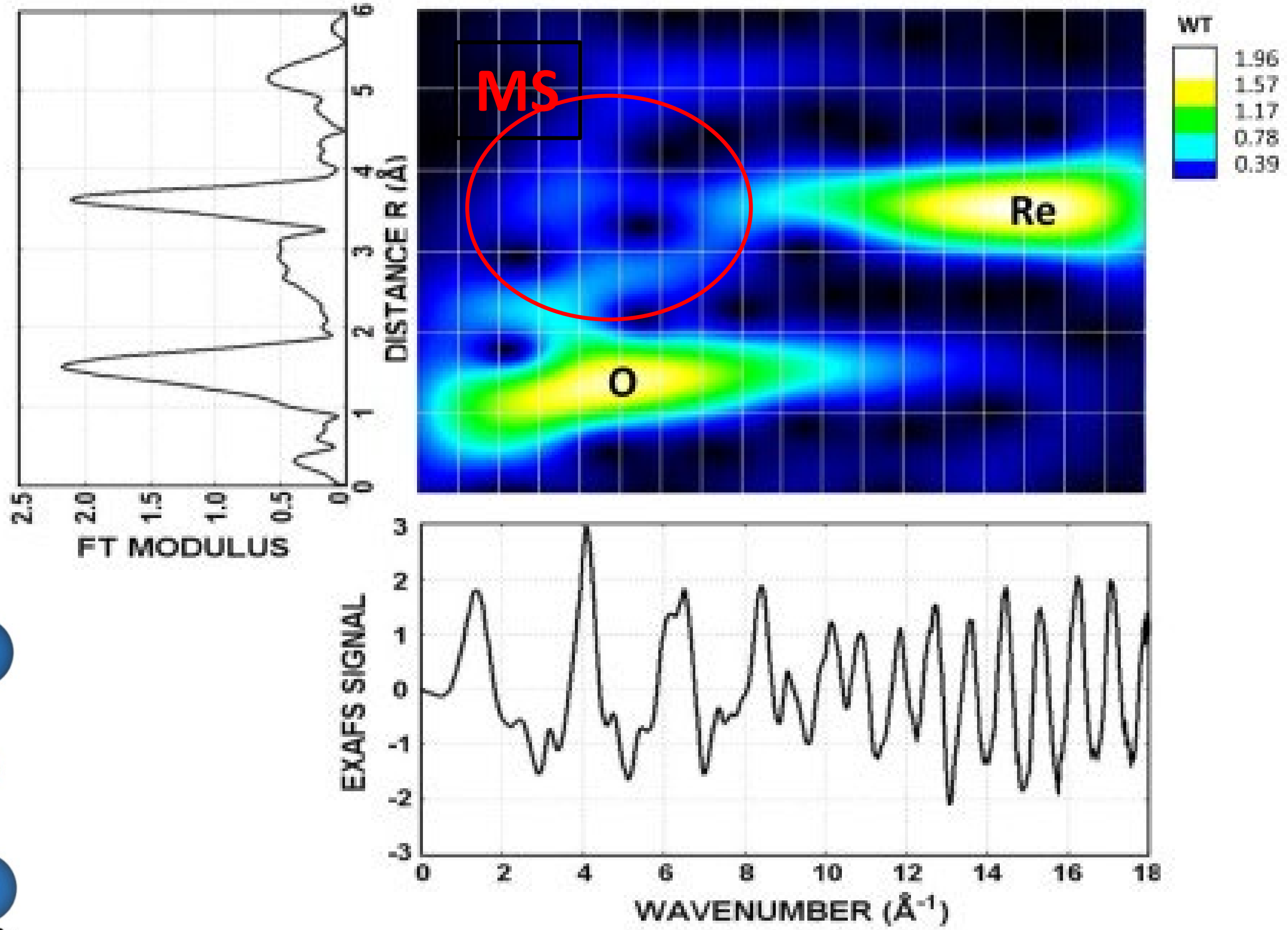
- It is invertible:

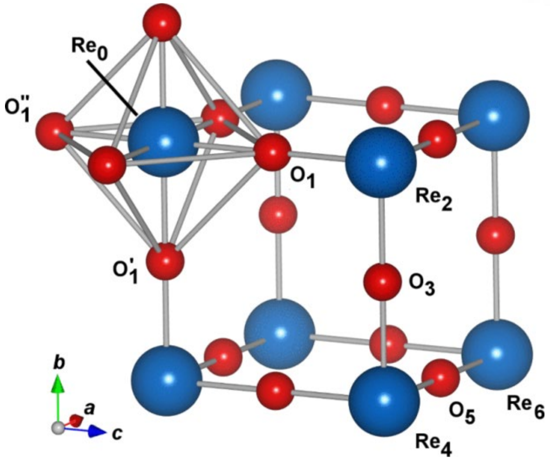
$$\chi(k) = \frac{1}{C} \int_{k_{min}}^{k_{max}} \int_{R_{min}}^{R_{max}} WT(k',R)\,(R/R_0)^{\frac{1}{2}} \phi^*\left(\frac{k'-k}{R_0/R}\right) \frac{dR}{R_0} dk'$$

$$C = \int_0^\infty \frac{\left|\hat{\phi}(R)\right|^2}{R} dR$$

WT-EXAFS: examples

Single-scattering and multiple-scattering effects in Re L_3-edge EXAFS spectra for ReO_3



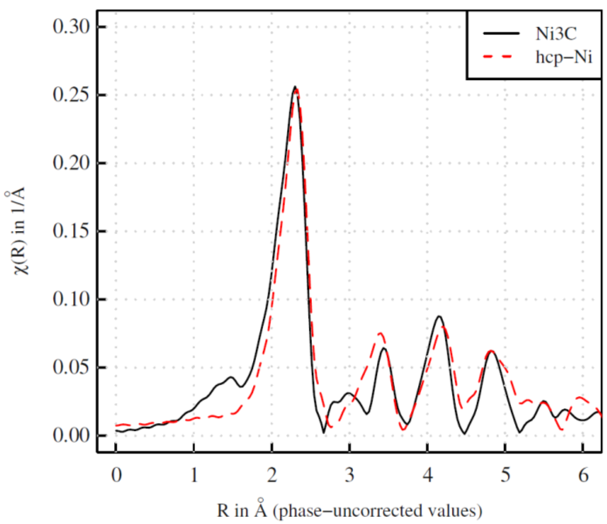


J Timoshenko, A Kuzmin – Comp.Phys. Commun. 180 (2009)

WT-EXAFS: examples

Discrimination of metallic and non-metallic species (hcp-Ni vs. Ni_3C)

Ni clusters in piezoresistive Ni:a-C:H thin films may assume fcc-Ni, hcp-Ni or Ni_3C, dependently on film deposition conditions. hcp-Ni and Ni_3C is very hard to distinguish by XRD, and also Ni-Ni EXAFS is very similar.



(b) Calculated $\chi(R)$ obtained by ATHENA, based on $\chi(k)$ data of Fig. 3a.

Fig. 3. Theoretical $\chi(k)$ and $\chi(R)$ spectra of hcp-Ni (JCPDS #00-045-1027) and Ni_3C (JCPDS #01-072-1467).

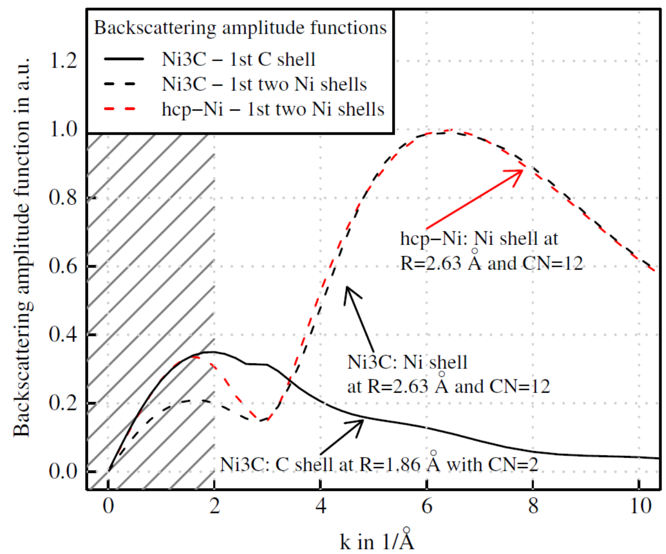
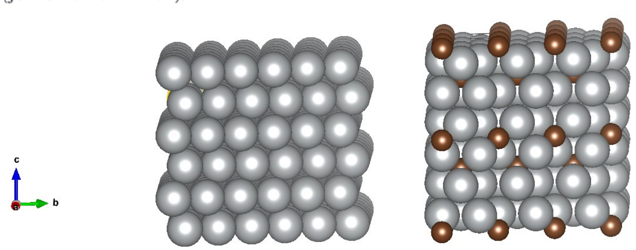


Fig. 4. Backscattering amplitude functions (BAF) of C and Ni with Ni_3C and that of Ni with hcp-Ni. Each BAF was calculated with FEFF6 by assuming single coordination shells with Ni and C, respectively. CN - coordination number.



Uhlig et al, Diamond & Related Materials 34 (2013)

WT-EXAFS: examples

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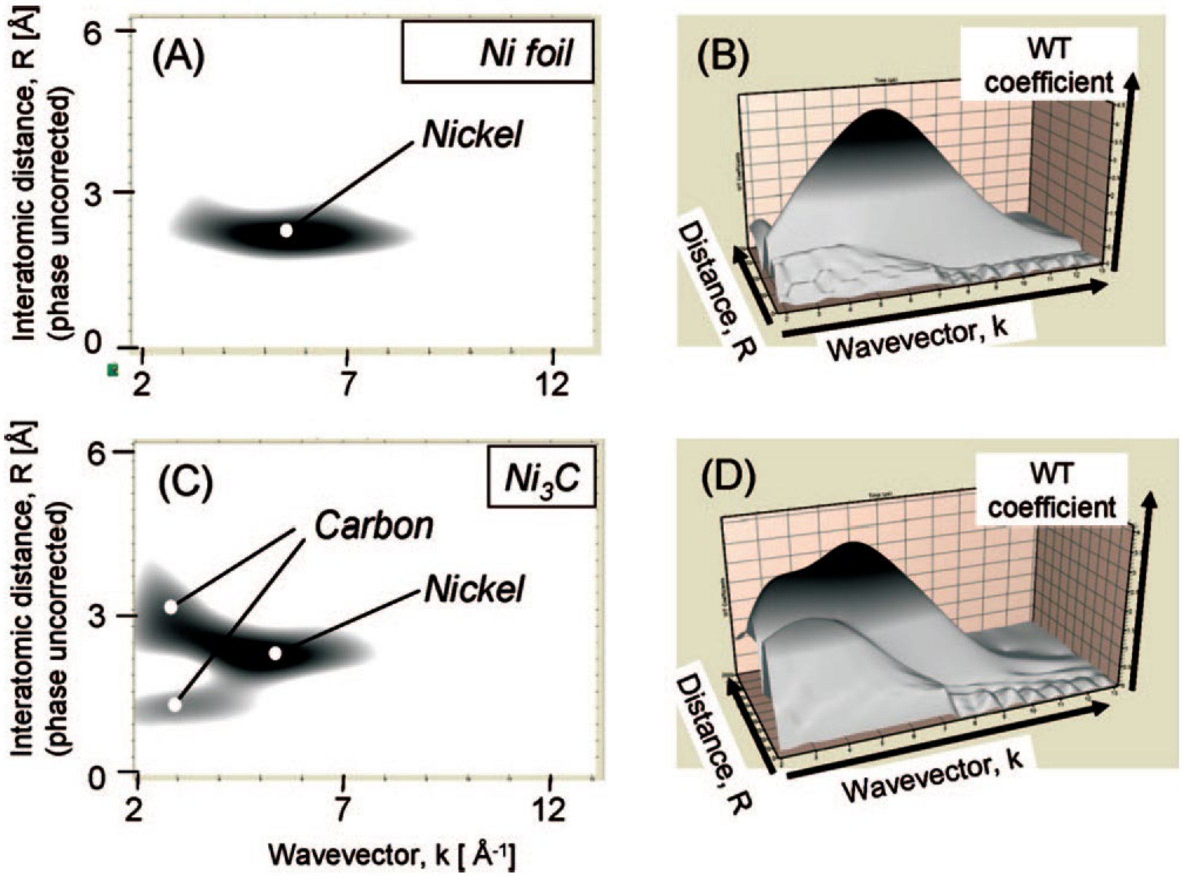
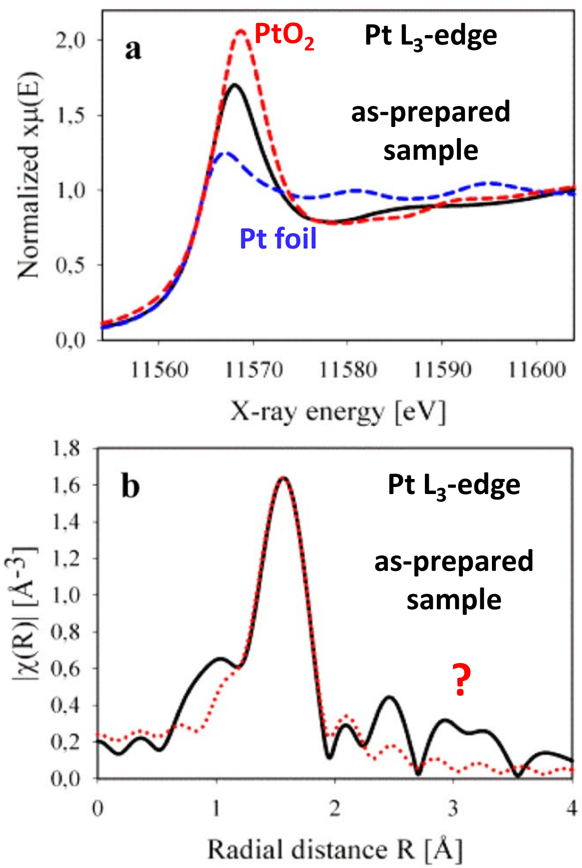


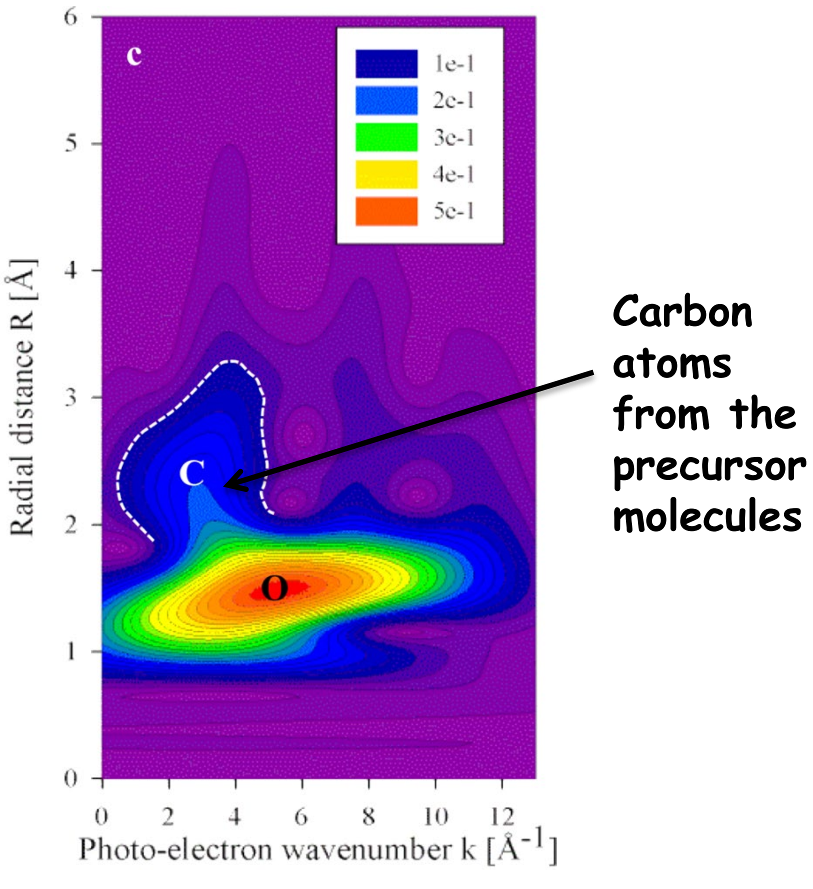
Struis et al, J. Phys. Chem. C 2009, 113

WT-EXAFS: examples

Analysis of multi-element compounds (Pt on Mg(In)(Al)O_x support)

1. Pt precursor (acetylacetonate) was impregnated on Mg(In)(Al)O_x mixed oxide. Analysis of first coordination shell is straightforward. But what are the distant peaks in FT-EXAFS?



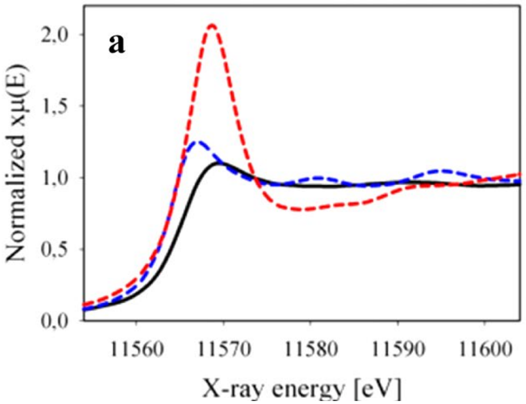


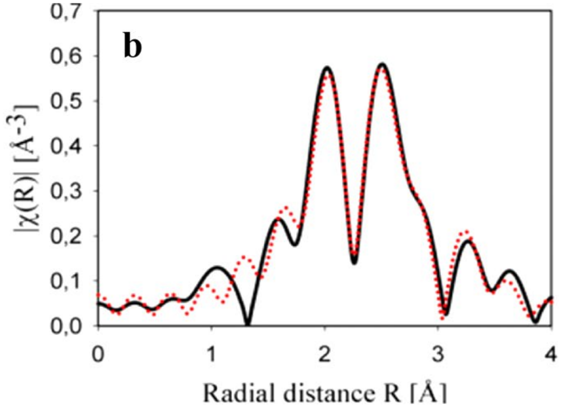
Filez et al, Analytical chemistry 87 (2015)

WT-EXAFS: examples

Analysis of multi-element compounds (Pt on Mg(In)(Al)O_x support)

3. After reduction in H_2/He to 650^0C

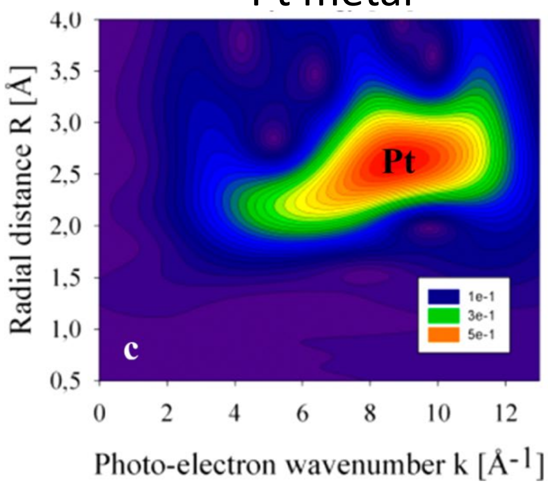




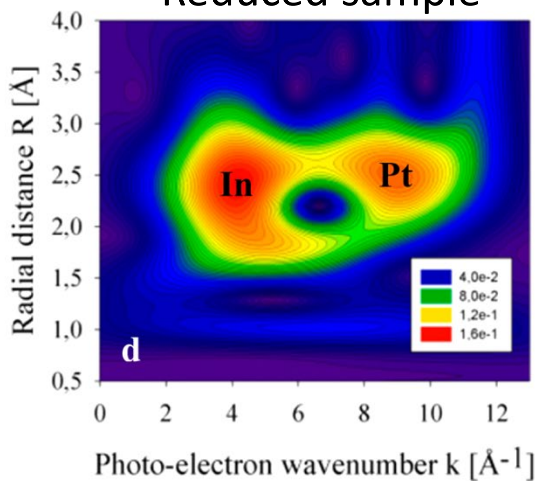
Pt-O feature has disappeared after reduction. But XANES does not look like that in metallic Pt…

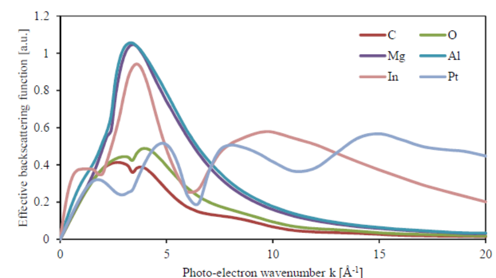
WT-EXAFS has Pt-Pt feature, but is different from that in metallic Pt: indicates alloying with In from the support.

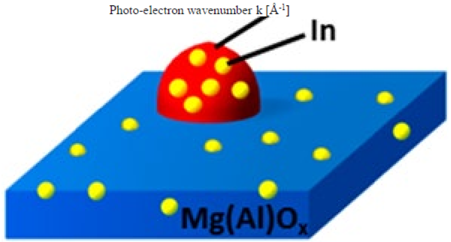
Pt metal



Reduced sample



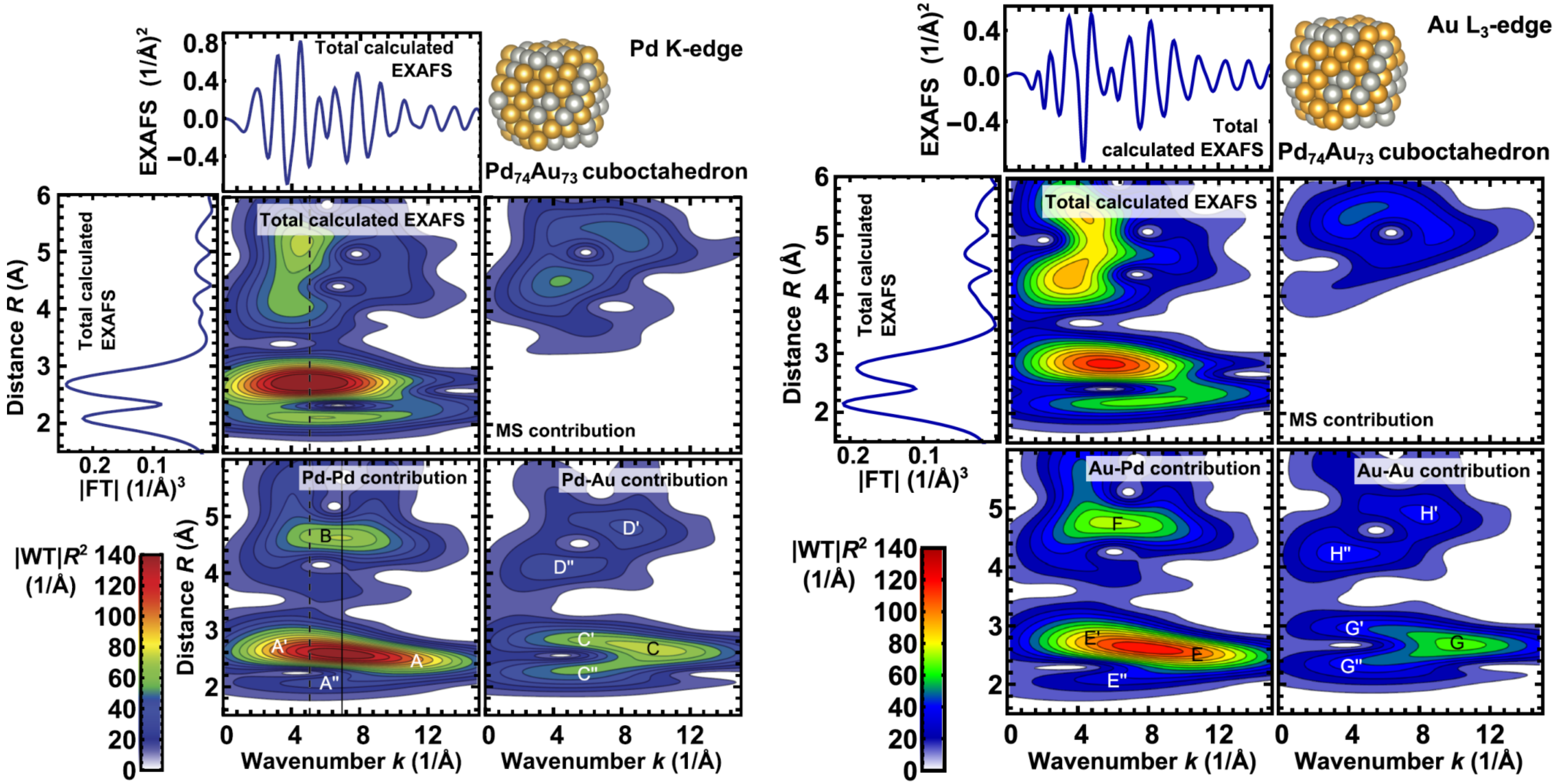




Filez et al, Analytical chemistry 87 (2015)

WT-EXAFS: examples

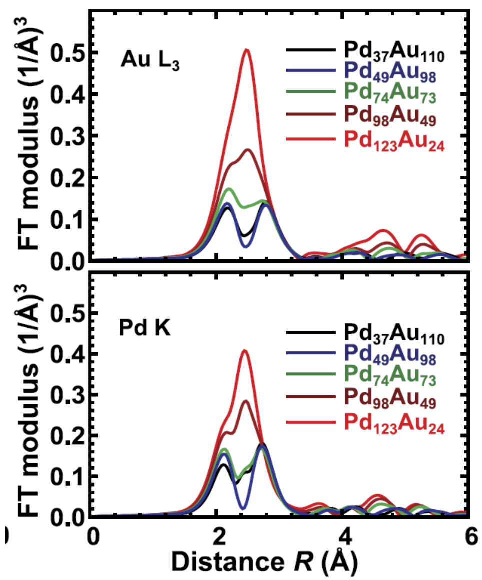
Analysis of bimetallic systems; Ramsauer-Townsend effect

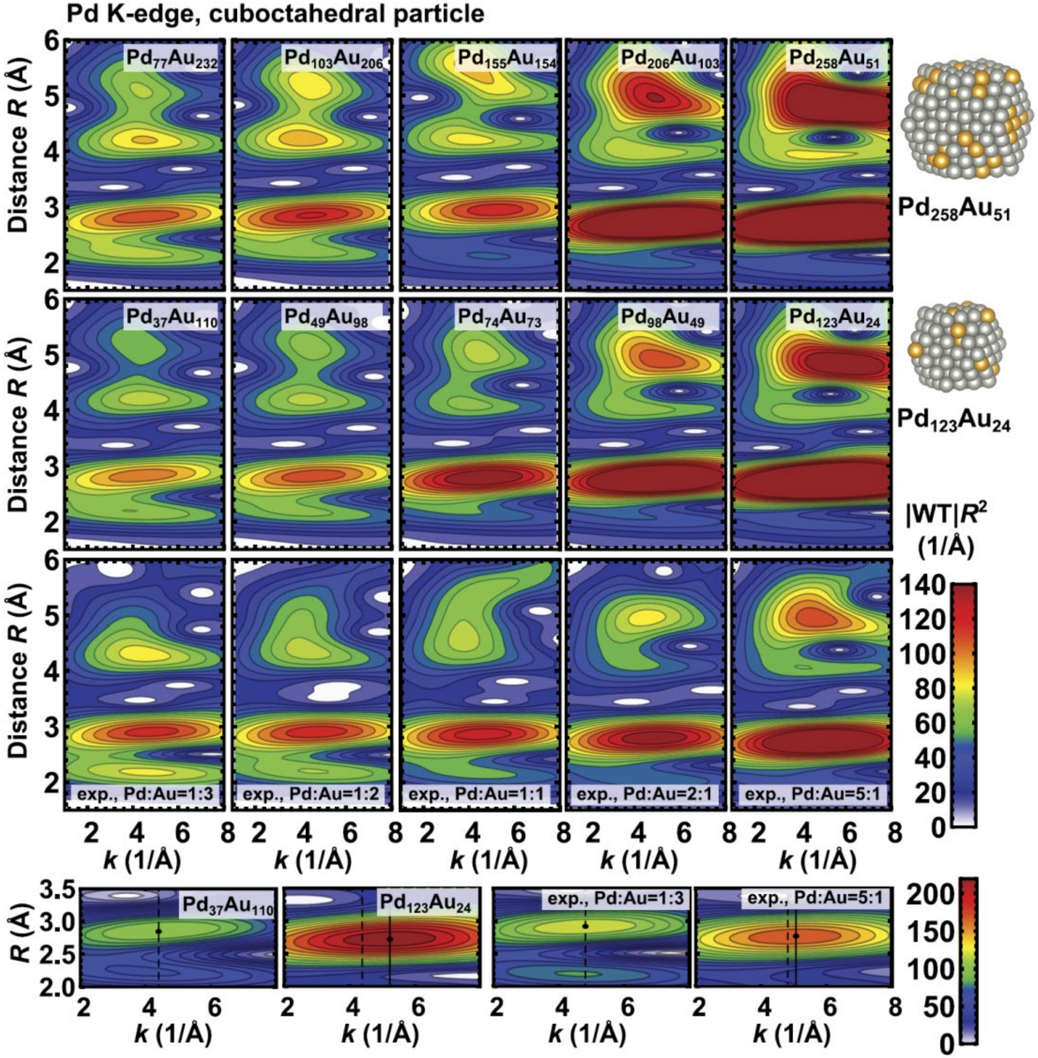


Timoshenko, Keller, Frenkel, J.Chem. Phys. 146 (2017)

WT-EXAFS: examples

Analysis of bimetallic systems; chemical sensitivity and size sensitivity

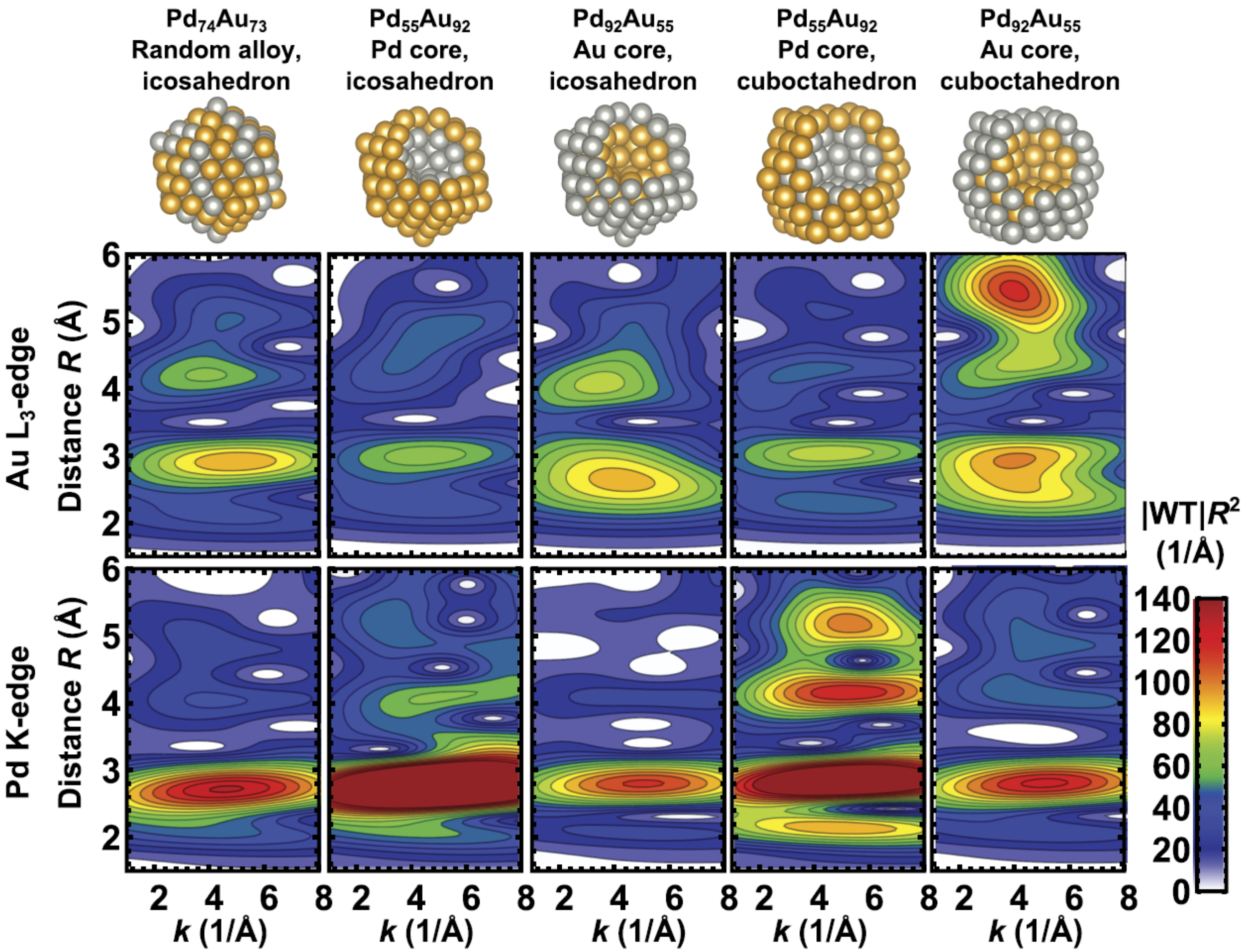




Timoshenko, Keller, Frenkel, J.Chem. Phys. 146 (2017)

WT-EXAFS: examples

Analysis of bimetallic systems; sensitivity to structural motifs



Timoshenko, Keller, Frenkel, J.Chem. Phys. 146 (2017)

Summary and conclusions

- Wavelet transform is an integral transformation, similar to Fourier transform, but provides information not only about signal frequencies, but also about the location of different spectral components in the original space.

- Wavelet transform provides a more informative way for visualization of EXAFS spectra: allows one to distinguish signal from artefacts, to discriminate between contributions of different species.

- Fitting of EXAFS data in wavelet space allows one to exploit more efficiently the information, encoded in EXAFS features, and may stabilize the fit.

Thank you for your attention!