Solving EXAFS puzzle using reverse Monte Carlo simulations

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https://www.facebook.com/EXAFSLab/

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UNIVERSITY OF LATVIA

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PSI

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Talk Outline

- **History of synchrotron radiation research in Latvia**
  - Experiments → Effects → Data analysis
- **Advanced methods for X-ray absorption spectra interpretation**
  - Effect of disorder & multiple-scattering (MS)
- **Reverse Monte Carlo (RMC) simulations**
  - Capabilities and limitations
  - Crystalline germanium
  - Lattice dynamics in 2D compounds
- **RMC applications to multicomponent materials**
  - $NiWO_4$-$ZnWO_4$ solid solutions
  - medium-entropy $(MnNiCuZn)WO_4$ and a high-entropy $(MnCoNiCuZn)WO_4$ tungstates
- **Conclusions**

Synchrotron radiation research in Latvia (I)

1982 - 93 | **1993 - 2006** | **2000 - …**

Juris Purans (1982)

A. Kuzmin (1985)
MS

(1997)
MD

J. Timoshenko (2006)
RMC/MD

A. Kalinko (2007)
MD/DFT

A. Anspoks (2009)
MD/RMC

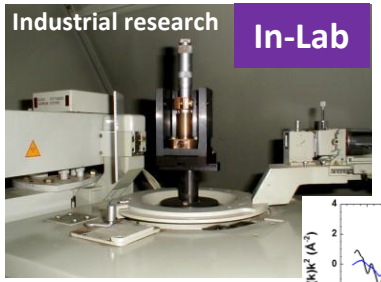
I. Jonane/Pudza (2013)
RMC/RIXS

LURE

ADONE

Electrochromic Thin Films & Glasses

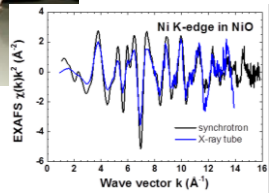
VEPP-4



In-Lab

1989-1997

DORIS III



PETRA III
Hamburg, Germany

MAX IV
Lund, Sweden

SOLEIL
Gif-sur-Yvette Cedex, France

ALBA
Cerdanyola del Vallès (Barcelona), Spain

Elettra
Trieste, Italy

ESRF
Grenoble, France

Synchrotron radiation research in Latvia (II)

1982 - 93 | **1993 - 2006** | **2000 - …**

J. Purans — FT/SS

A. Kuzmin (1985) — MS

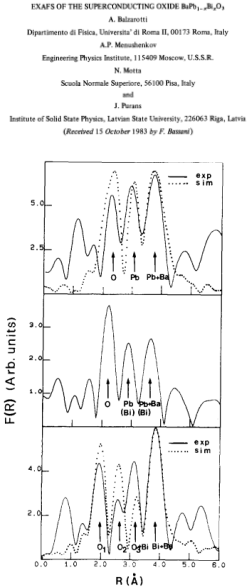
(1997) — MD

J. Timoshenko (2006) — RMC

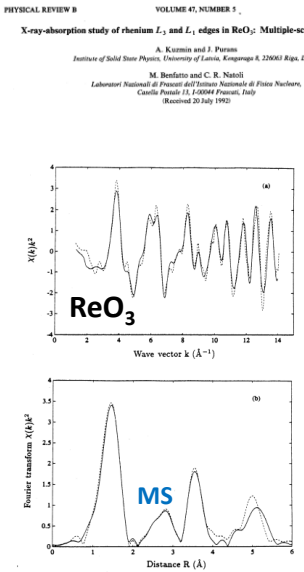
A. Kalinko (2007) — MD/DFT

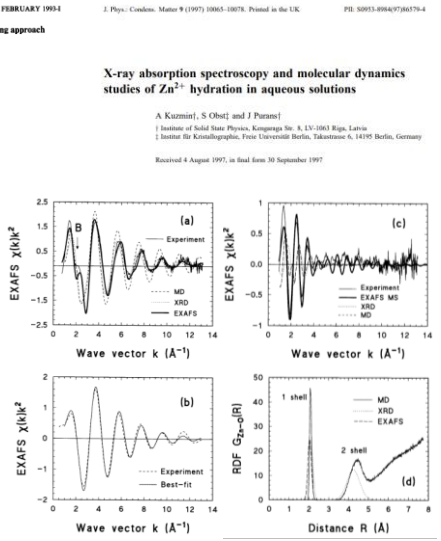
A. Anspoks (2009) — MD

I. Jonane/Pudza (2013) — RMC/RXES



DEC VAX / Intel 8086/286





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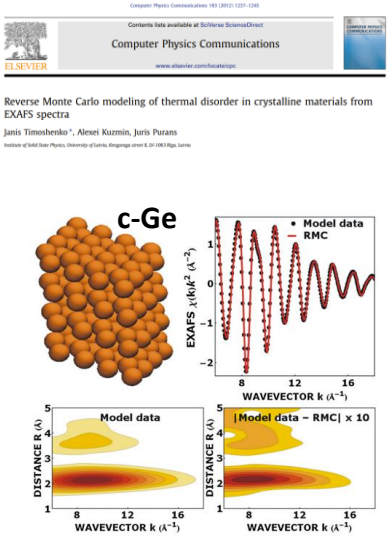

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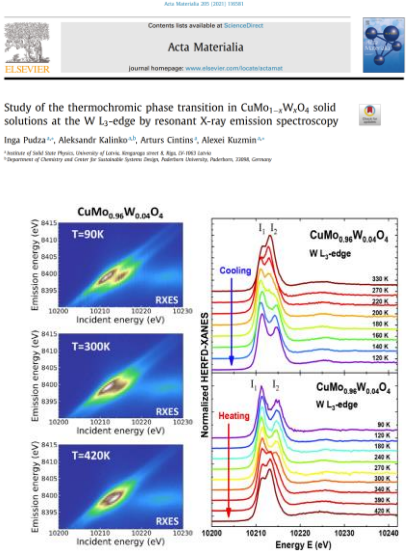

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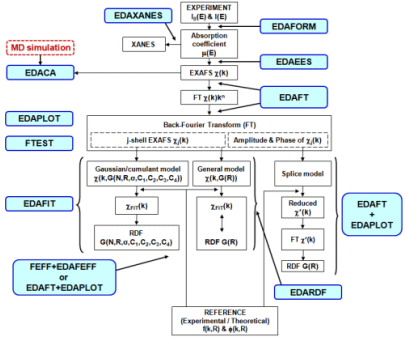
XAS data analysis in Latvia

EXAFS analysis

EDA
EXAFS DATA ANALYSIS
Software Package



A. Kuzmin,
Physica B 208&209 (1995) 175-176.

Molecular Dynamics + EXAFS (MD-EXAFS)

EDACA

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Preface

X-ray absorption spectroscopy (XAS) at synchrotron radiation sources is a structural tool providing information on the local atomic and electronic structure around an atom of a particular type. Today XAS is successfully applied to a study of crystalline, nanocrystalline and disordered solids, liquids and gases in a wide range of external conditions defined by temperature, pressure, etc. The size of the region, probed by XAS, depends on the degree of thermal and static disorder present in a material and is limited by the mean-free path of the excited photoelectron. Typically the information reach region extended up to 3-10 A around the absorbing atom.

An advantage of the XAS method is its sensitivity to many-atom distribution functions, giving rise to multiple-scattering (MS) contributions, and to correlation effects in atom dynamics. Note that accurate account of both effects is still challenging.

The time-scale (about 10^{-15}-10^{-16} s) of the X-ray absorption process is much shorter than the characteristic time (about 10^{-13}-10^{-14} s) of thermal vibrations. Therefore, the atoms may be considered as frozen at their instantaneous positions during a single photoabsorption process, and the total experimentally measured X-ray absorption spectrum corresponds to the configurational average of all atomic positions over the time of the experiment. This situation can be straightforwardly modelled combining the molecular dynamics (MD) simulation with the extended X-ray absorption fine structure (EXAFS) calculations, known as the MD-EXAFS approach.

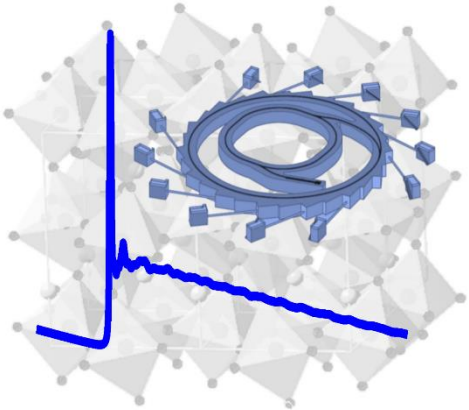
Finally, the agreement between the experimental and configuration-averaged EXAFS spectra can be used to validate the accuracy of the interatomic potential (force-field) models employed in the MD simulations.

A. Kuzmin and R.A. Evarestov,
J. Phys.: Condens. Matter 21 (2009) 055401.

Reverse Monte Carlo (RMC) with Evolutionary Algorithm

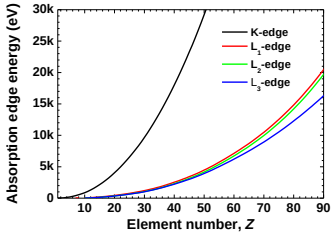
J. Timoshenko, A. Kuzmin, J. Purans,
J. Phys.: Condens. Matter 26 (2014) 055401.

Advanced methods for X-ray absorption spectra interpretation



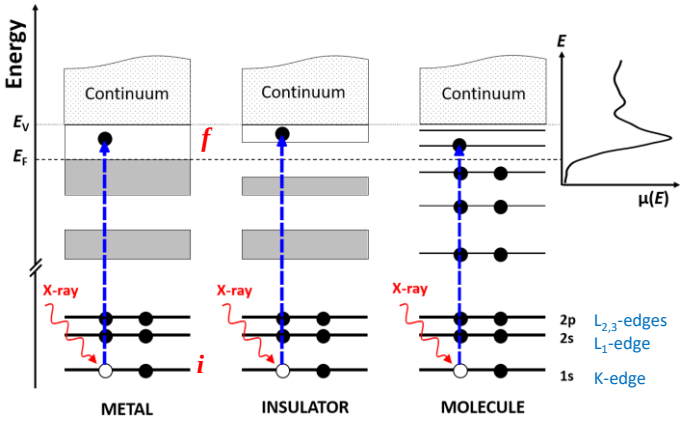
Basics of X-ray absorption spectroscopy (XAS)

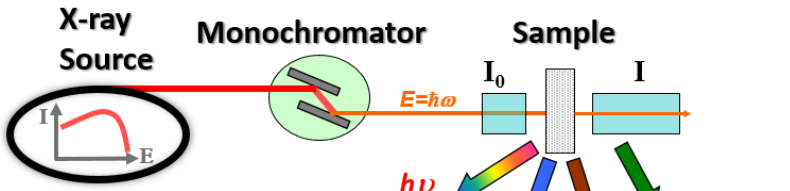
X-rays:
soft (<5 keV)
hard (>5 keV)

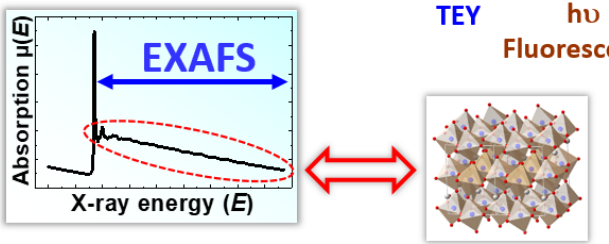


Fermi's Golden Rule:

$$\mu(E) \propto \sum_f \left|\langle f|\hat{\mathbf{H}}|i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega)$$







$$\mu(E) = \frac{1}{x}\ln\left(\frac{I_0(E)}{I(E)}\right)$$

$$\mu(E) \propto \frac{I_{\text{fluo}}(E)}{I_0(E)}$$

$$\mu(E) \propto \frac{I_{\text{TEY}}(E)}{I_0(E)}$$

$$\mu(E) \propto \frac{I_{\text{XEOL}}(E)}{I_0(E)}$$

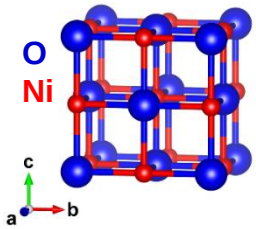
Characteristic time of X-ray absorption process:

$t_{ab} \sim 10^{-15}$-10^{-16} s

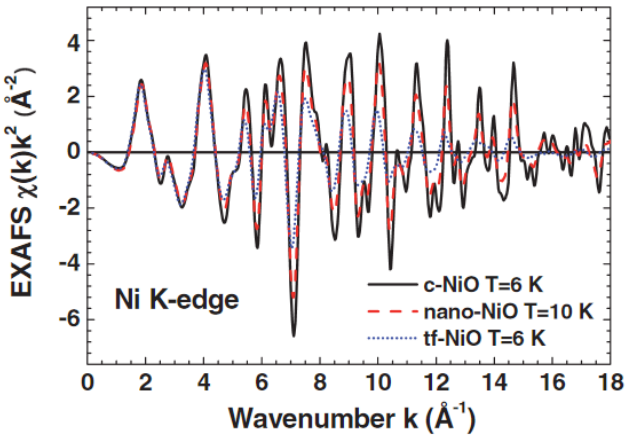
Characteristic time of thermal vibrations:

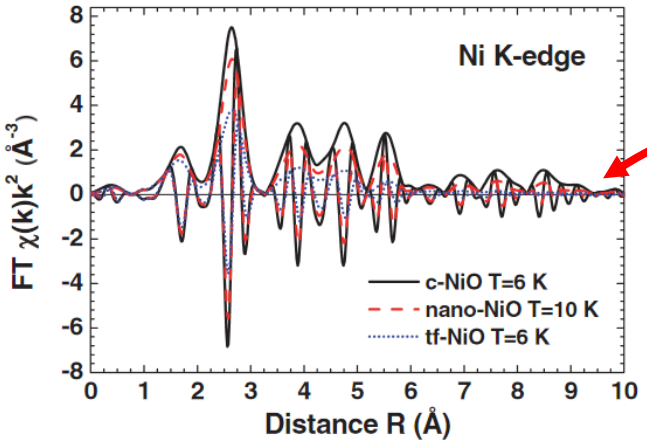
$t_{th} \sim 10^{-13}$-10^{-14} s

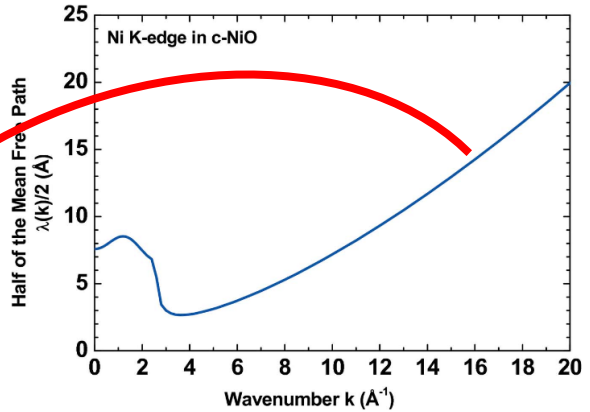
- **Atoms are frozen during X-ray absorption**
- **Static & thermal disorder contribute similarly**



How local is X-ray absorption spectroscopy?
The case of NiO: T = ~10 K



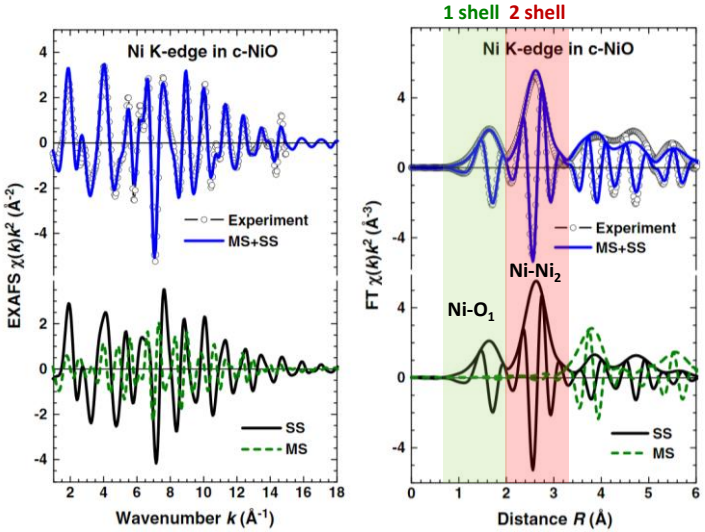




A. Anspoks, A. Kalinko, R. Kalendarev, A. Kuzmin, Phys. Rev. B 86 (2012) 174114.

EXAFS challenges: analysis of distant coordination shells

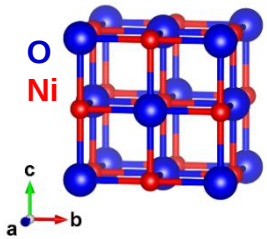
1 The analysis of the distant coordination shells must take into account the multiple-scattering (MS) and disorder effects.



A. Anspoks and A. Kuzmin,
J. Non-Cryst. Solids 357 (2011) 2604.

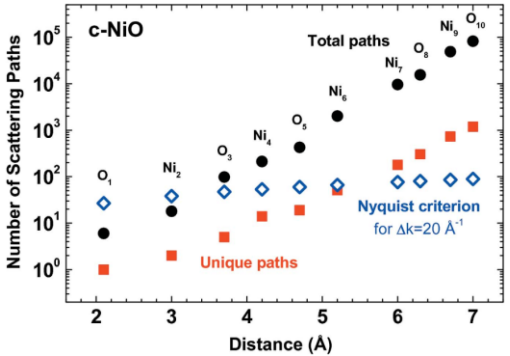
NiO

Space group Fm-3m
a_0 = 4.1773 Å



2 A number of parameters in the model increases rapidly upon an increase of analyzed region size around the absorbing atom.

This problem is especially relevant for disordered and nanocrystalline materials.



Number of scattering paths vs independent parameters N_{par}:

$$N_{\mathrm{par}} = \frac{2\Delta k \Delta R}{\pi}$$

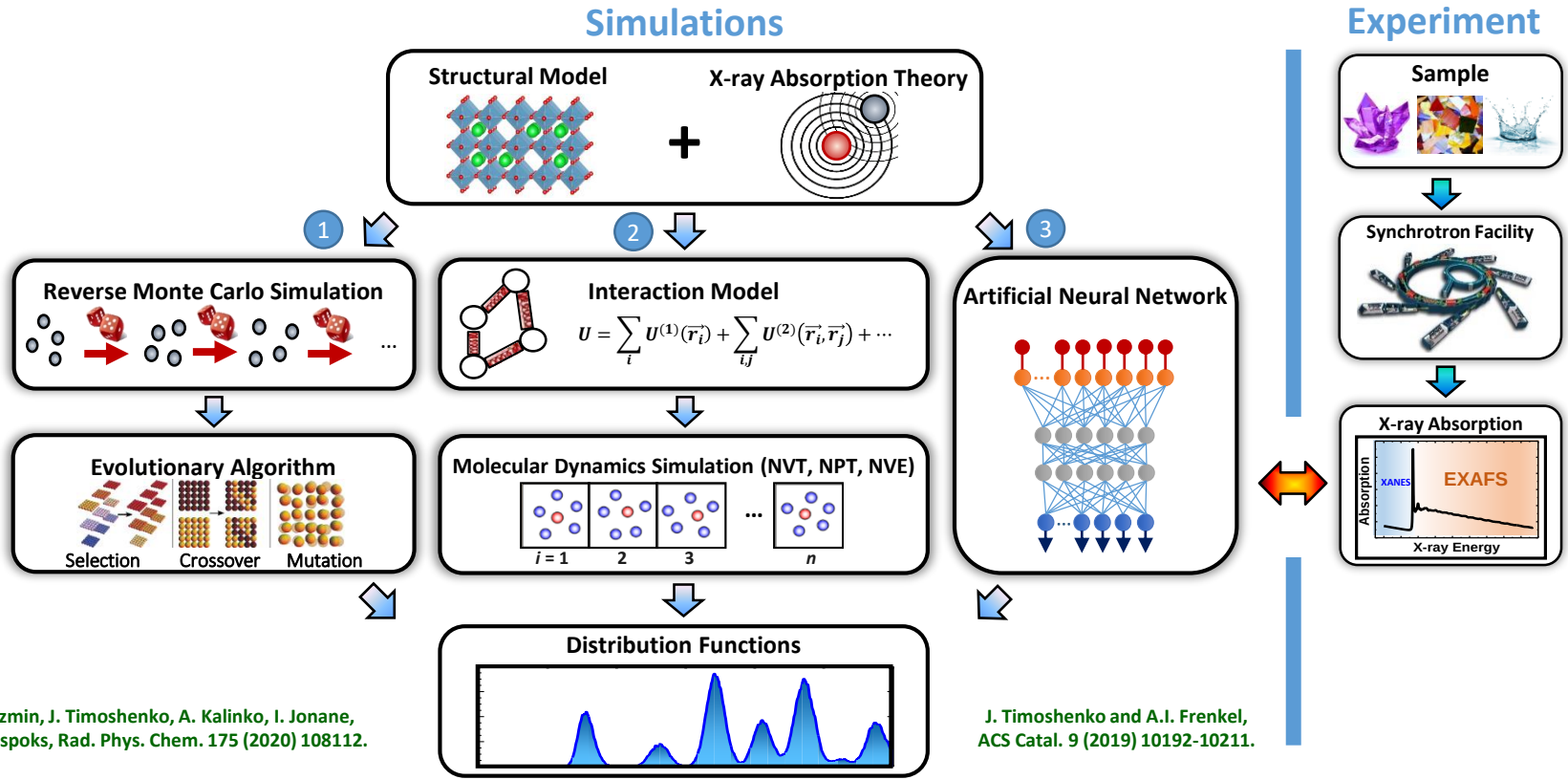
A. Kuzmin and J. Chaboy, IUCrJ 1 (2014) 571.

Why do we need advanced methods of EXAFS analysis?

- To account properly for disorder effects.
- To perform reliable analysis of distant coordination shells.
- To determine bond-angle distribution functions.
- To extract structural information in some specific cases (nanoparticles).
- To validate other theoretical simulations as molecular dynamics or DFT calculations.

[1] A. Kuzmin and J. Chaboy, EXAFS and XANES analysis of oxides at the nanoscale, IUCrJ 1 (2014) 571.
[2] A. Kuzmin, J. Timoshenko, A. Kalinko, I. Jonane, A. Anspoks, Treatment of disorder effects in X-ray absorption spectra beyond the conventional approach, Rad. Phys. Chem. 175 (2020) 108112.

Advanced methods of XAS analysis using atomistic simulations



A. Kuzmin, J. Timoshenko, A. Kalinko, I. Jonane, A. Anspoks, Rad. Phys. Chem. 175 (2020) 108112.

J. Timoshenko and A.I. Frenkel, ACS Catal. 9 (2019) 10192-10211.

Reverse Monte Carlo (RMC) method: 1st paper

Molecular Simulation, 1988, Vol. 1, pp. 359–367
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REVERSE MONTE CARLO SIMULATION: A NEW TECHNIQUE FOR THE DETERMINATION OF DISORDERED STRUCTURES

R.L. MCGREEVY

Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK

L. PUSZTAI

Laboratory of Theoretical Chemistry, Department of Chemistry, L. Eotvos University, H-1088 Budapest, Hungary

(*Received March 1988*)

We have developed a new technique, based on the standard Monte Carlo simulation method with Markov chain sampling, in which a set of three dimensional particle configurations are generated that are consistent with the experimentally measured structure factor, A(Q), and radial distribution function, g(r), of a liquid or other disordered system. Consistency is determined by a standard χ^2 test using the experimental errors. No input potential is required, we present initial results for liquid argon. Since the technique can work directly from the structure factor it promises to be useful for modelling the structures of glasses or amorphous materials. It also has other advantages in multicomponent systems and as a tool for experimental data analysis.

Radial Distribution Function

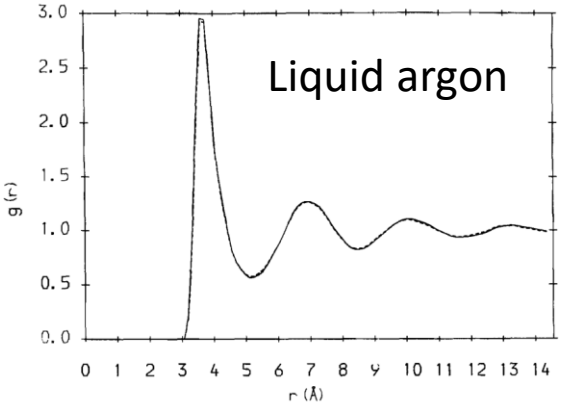


Figure 1 Radial distribution function g(r) for liquid argon; comparison of experiment [3] (solid line) and RMC calculation (broken line).

Structure factor

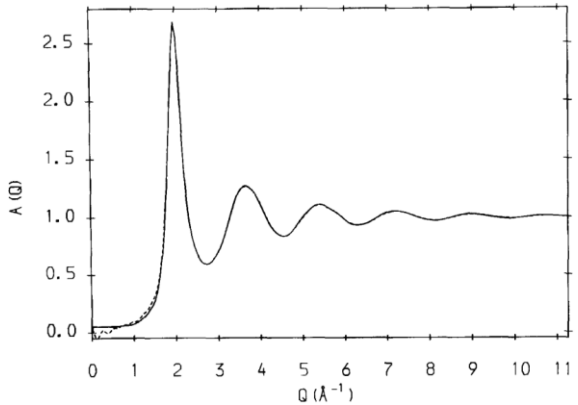


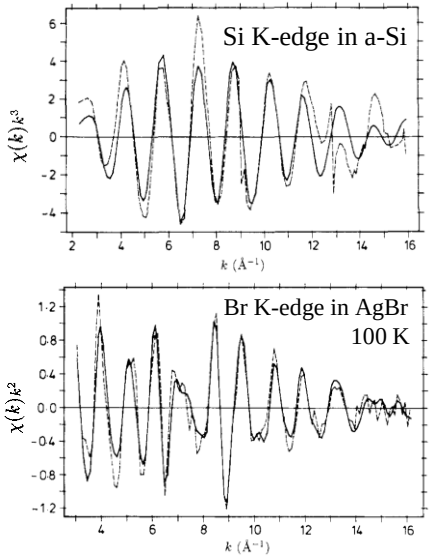
Figure 2 Structure factor A(Q) for liquid argon; comparison of experiment [3] (solid line) and RMC calculation (broken line).

R. L. McGreevy & L. Pusztai, Reverse Monte Carlo Simulation: A New Technique for the Determination of Disordered Structures, Molecular Simulation, 1 (1988) 359-367.

RMC-EXAFS approach: Earlier works

Reverse Monte Carlo simulation for the analysis of EXAFS data

S J Gurman† and R L McGreevy‡
† Department of Physics, University of Leicester, Leicester LE1 7RH, UK
‡ Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK



High temperature EXAFS experiments on liquid KPb alloys analysed with the reverse Monte Carlo method

W. Bras [a,b,*], R. Xu [c], J.D. Wicks[d,1], F. van der Horst [c], M. Oversluizen [a,b], R.L. McGreevy [c], W. van der Lugt [c]
[a] Netherlands Organisation for Scientific Research (NWO), The Netherlands
[b] SERC Daresbury Laboratory, Warrington WA4 4AD, UK
[c] Laboratory for Solid State Physics, Groningen University, Nijenborgh 18, 9747 AG Groningen, The Netherlands
[d] Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK
[e] Studsvik Neutron Research Laboratory, Uppsala University, S-611 82 Nyköping, Sweden

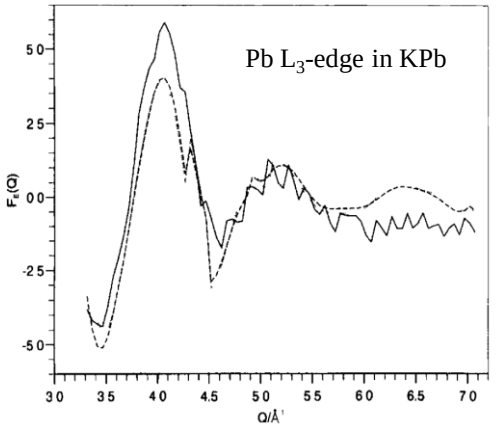
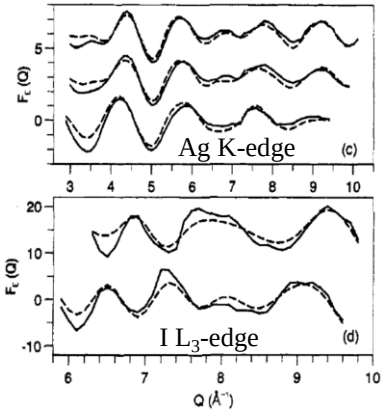


Fig. 4. EXAFS data, $F_L(Q)$, for molten KPb (solid line) compared to the RMC fit with 100% Zintl ions maintained (dotted line)

Modelling the Structure and Ionic Conduction of $(AgI)_x(AgPO_3)_{1-x}$ Glasses

J. D. Wicks,[1] L. Börjesson,[2] G. Bushnell-Wye,[3] W. S. Howells,[4] and R. L. McGreevy[5]
[1] Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, U.K.
[2] Department of Physics, Royal Institute of Technology, S-100 44 Stockholm, Sweden
[3] SRS Daresbury Laboratory, Warrington, Cheshire WA4 4AD, U.K.
[4] ISIS Science Division, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, U.K.
[5] Studsvik Neutron Research Laboratory, S-611 82 Nyköping, Sweden



Experimental data (solid curves) and RMC fits (broken curves) for $(AgI)_x(AgPO_3)_{1-x}$ (top to bottom) x = 0.5, 0.3 and 0.0. EXAFS at (c) the Ag K-edge and (d) the I L_3-edge.

[1] S.J. Gurman and R.L. McGreevy, J. Phys.: Condens. Matter 2 (1990) 9463-9473.
[2] W. Bras, R. Xu, J.D. Wicks, F. van der Horst, M. Oversluizen, R.L. McGreevy, W. van der Lugt, Nucl. Instrum Meth. Phys. Res. A 346 (1994) 394-398.
[3] J.D. Wicks, L. Borjesson, G. Bushnell-Wye, W.S. Howells, R.L. McGreevy, Physica Scripta. T57 (1995) 127-132.

Available software for RMC-EXAFS simulations

RMC-GNXAS [1], RMCprofile [2], RMC++/RMC_POT++ [3], EvAX [4]

[1] A. Di Cicco, A. Trapananti, J. Phys. Condens. Matter 17 (2005) S135.
[2] M.G. Tucker, D.A. Keen, M.T. Dove, A.L. Goodwin, Q. Hui, J. Phys.: Condens. Matter 19 (2007) 335218.
[3] O. Gereben, L. Pusztai, J. Computat. Chem. 33 (2012) 2285.
[4] J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter 26 (2014) 055401.

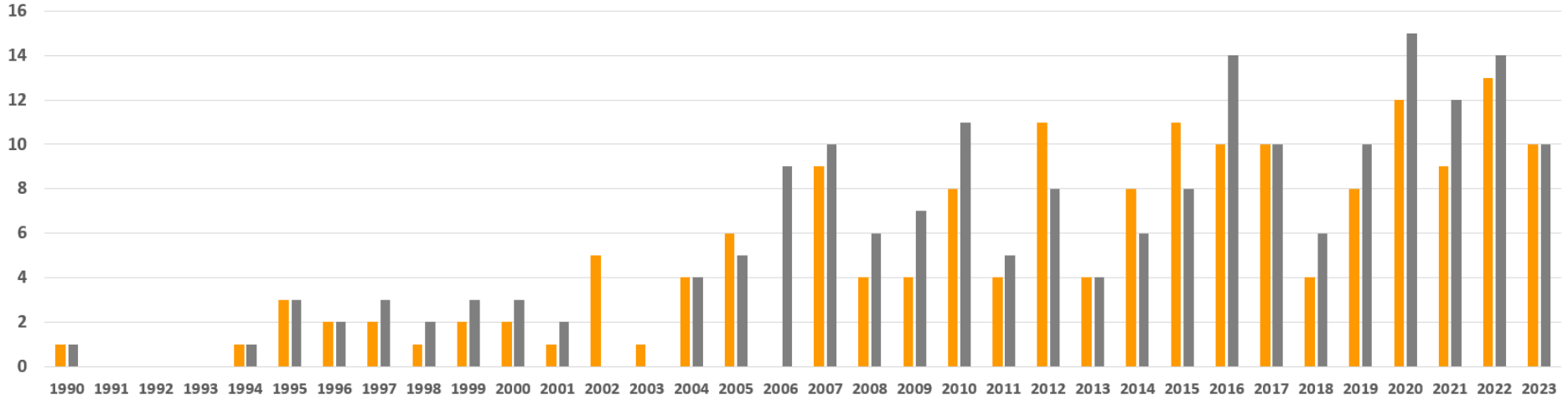
SpecSwap-RMC [5], EPSR-RMC [6]

[5] M. Leetmaa, K.T. Wikfeldt, L.G.M. Pettersson, J. Phys.: Condens. Matter 22 (2010) 135001.
[6] D.T. Bowron, Pure Appl. Chem. 80 (2008) 1211.

rmcxas [7]

[7] M. Winterer, J. Appl. Phys. 88 (2000) 5635.

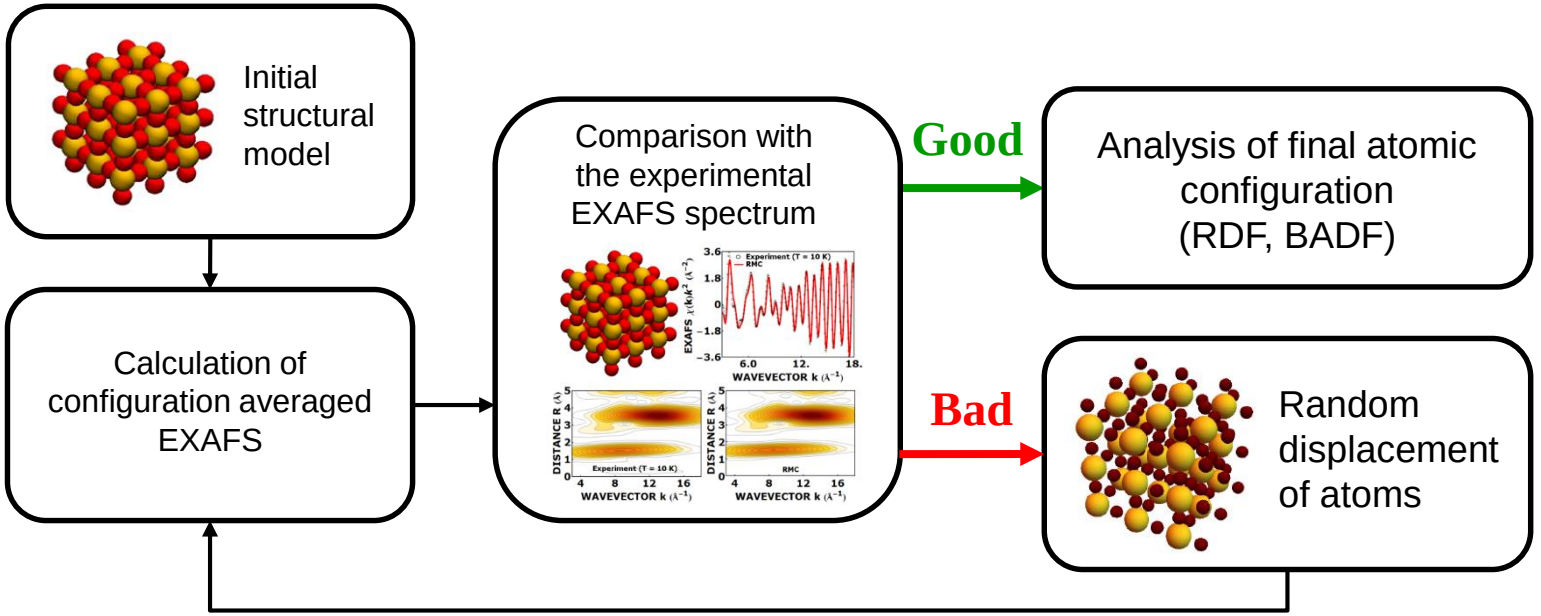
Publications on reverse Monte Carlo simulations of EXAFS



Scopus 170

Clarivate Web of Science™ 194

Reverse Monte Carlo simulations of EXAFS spectra (RMC-EXAFS)

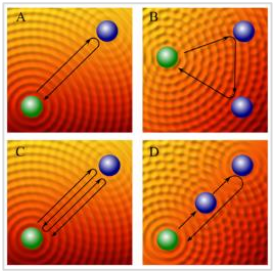


[1] R.L. McGreevy and L. Pusztai, Mol. Simul. 1 (1988) 359.
[2] J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter 26 (2014) 055401.

Reverse Monte Carlo method with Evolutionary Algorithm

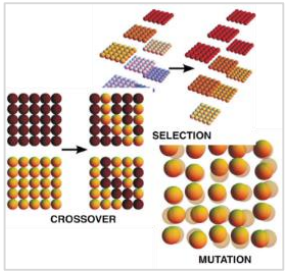
EvAX code was developed by Dr. Janis Timoshenko

J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter 26 (2014) 055401.
J. Timoshenko, A. Kuzmin, J. Purans, Comp. Phys. Commun. 183 (2012) 1237-1245.



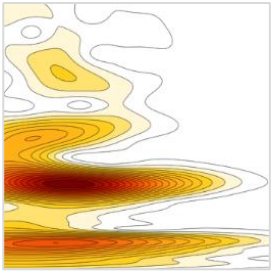
Multiple-scattering approximation

Reliable analysis of distant shells, PDF and BADF



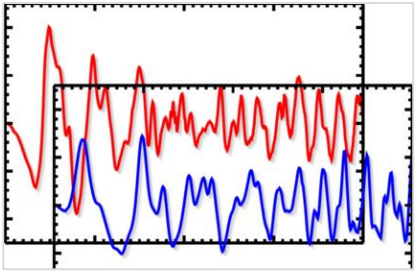
Evolutionary algorithm for optimization

Fast with good convergence



Wavelet transform for spectra comparison in k and R space

More reliable solution



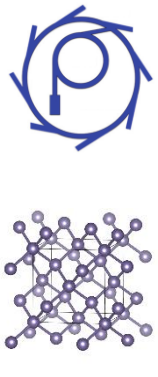
EXAFS spectra at several edges

One structural model

http://www.dragon.lv/evax/

Reverse Monte Carlo (RMC) simulation using the EvAX code

http://www.dragon.lv/evax/



*.cif

Experimental EXAFS spectrum

+

Starting structural model (supercell) (*.p1 file)

+

EvAX input file with commands

EvAX.exe -example

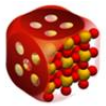
+

FEFF code

FEFF85L code

https://feff.phys.washington.edu/

RMC



Output files:

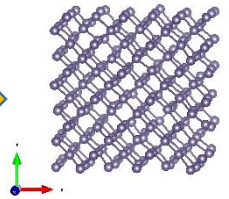
Log file

EXAFS
partial EXAFS
FT
WT

initial.xyz
final.xyz

restart

Gnuplot scripts for visualisation



RDF
BADF
MSRD
MSD

J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter 26 (2014) 055401.

Fourier and wavelet transforms of EXAFS $\chi(k)$

Fourier transform:

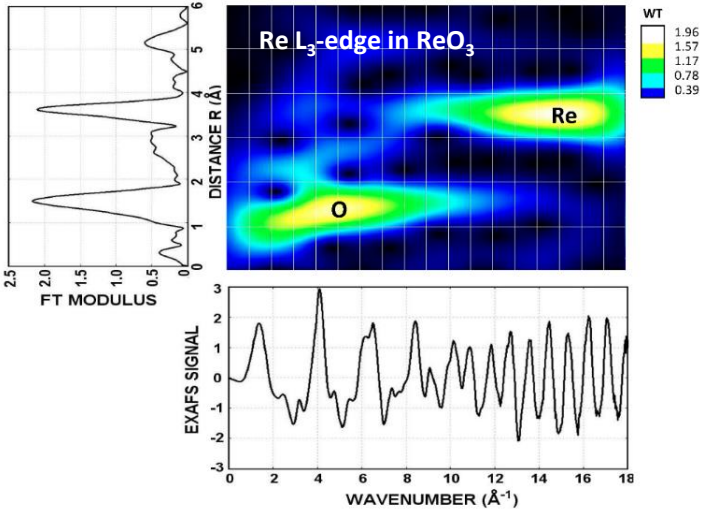
$$\mathrm{FT}(R) = \sqrt{\frac{2}{\pi}} \int_{k_{min}}^{k_{max}} k^n \chi(k) W(k) e^{-2ikR} dk$$

$W(k)$ is the window function

Wavelet transform:

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

$\phi(k) = e^{-2ikR_0} e^{-k^2/\sigma_0^2}$ is the Morlet wavelet



Fourier transform is a **1-dimensional integral transformation** providing information on the EXAFS signal behavior in ***R*-space**.

Wavelet transform is a **2-dimensional integral transformation** providing information on the EXAFS signal behavior in both ***k* and *R* spaces**.

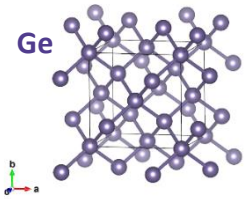
J. Timoshenko and A. Kuzmin, Wavelet data analysis of EXAFS spectra, Comp. Phys. Commun. 180 (2009) 920-925.

RMC simulations using the EvAX code for crystalline Ge

Calculation time for this example is about 6 min on 6-core CPU.

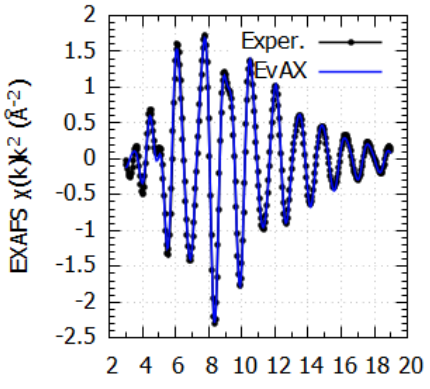
Crystalline Germanium:

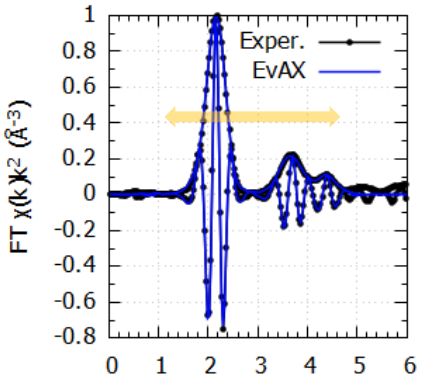
Lattice constant:
a = 5.657 Å
Space group Fd-3m

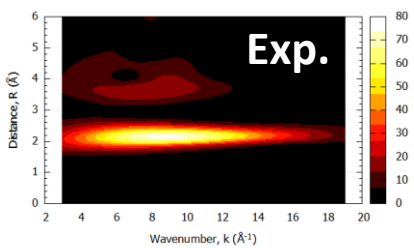


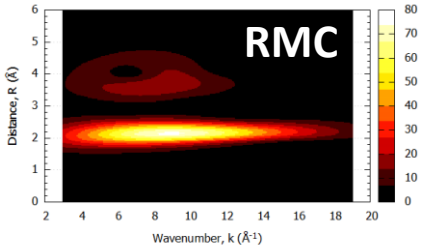
R(Ge-Ge):
4 x 2.45 Å
12 x 4.00 Å
12 x 4.69 Å

EvAX fit c-Ge T=300K

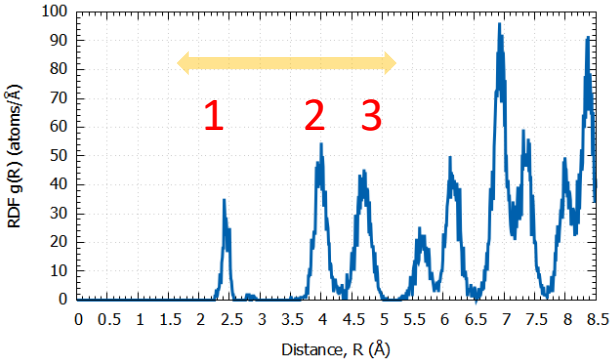








RMC supercell: 3 x 3 x 3



R_1 = 2.46 Å
$MSRD_1$ = 0.0037 Å²

R_2 = 4.00 Å
$MSRD_2$ = 0.011 Å²

R_3 = 4.69 Å
$MSRD_3$ = 0.014 Å²

MSD = 0.02 Å²

R_1(XRD)= 2.4497 Å

R_2(XRD)= 4.0039 Å

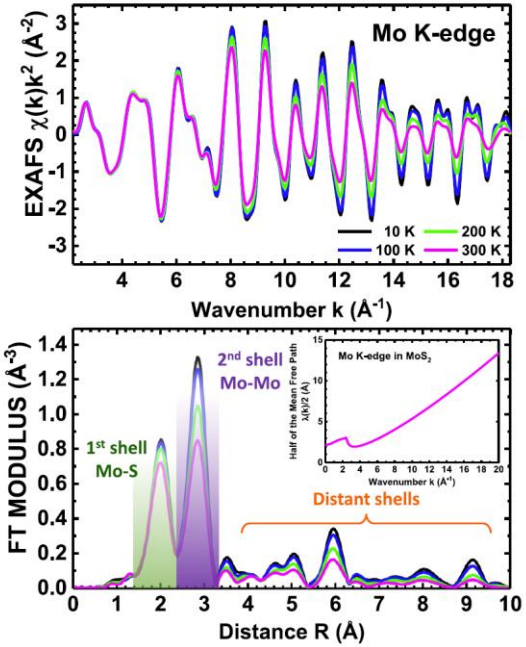
R_3(XRD)= 4.6909 Å

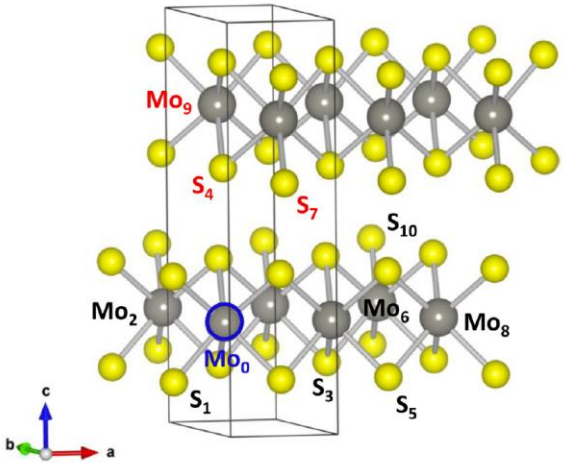
MSD(XRD)=0.022 Å²

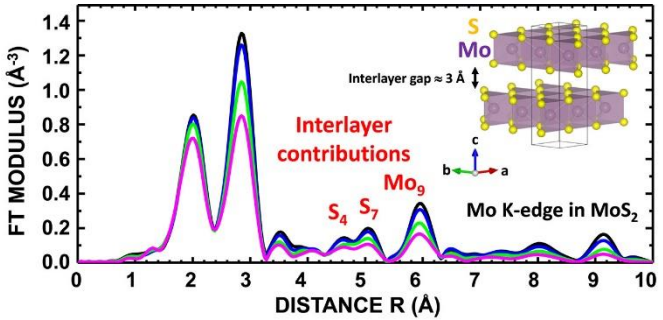
J. Timoshenko, A. Kuzmin, J. Purans, Reverse Monte Carlo modelling of thermal disorder in crystalline materials from EXAFS spectra, Comp. Phys. Commun. 183 (2012) 1237-1245.

N. M. Butt et al., Acta Crystallogr. A 44, 396 (1988).

Unraveling the interlayer and intralayer coupling in two-dimensional layered MoS_2

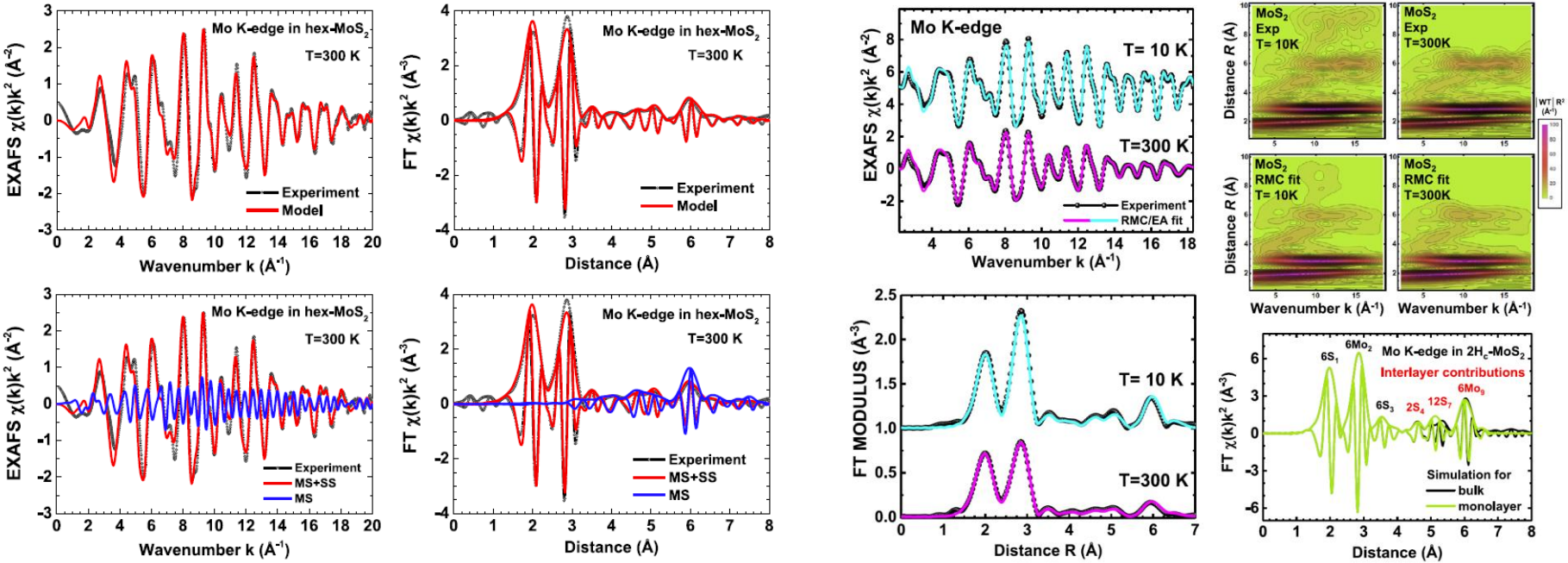






I. Pudza, D. Bocharov, A. Anspoks, M. Krack, A. Kalinko, E. Welter, A. Kuzmin, Mater. Today Commun. 35 (2023) 106359.

Unraveling the interlayer and intralayer coupling in two-dimensional layered MoS_2



Ab initio MD simulation **RMC fit**

I. Pudza, D. Bocharov, A. Anspoks, M. Krack, A. Kalinko, E. Welter, A. Kuzmin, Mater. Today Commun. 35 (2023) 106359.

Unraveling the interlayer and intralayer coupling in two-dimensional layered MoS_2

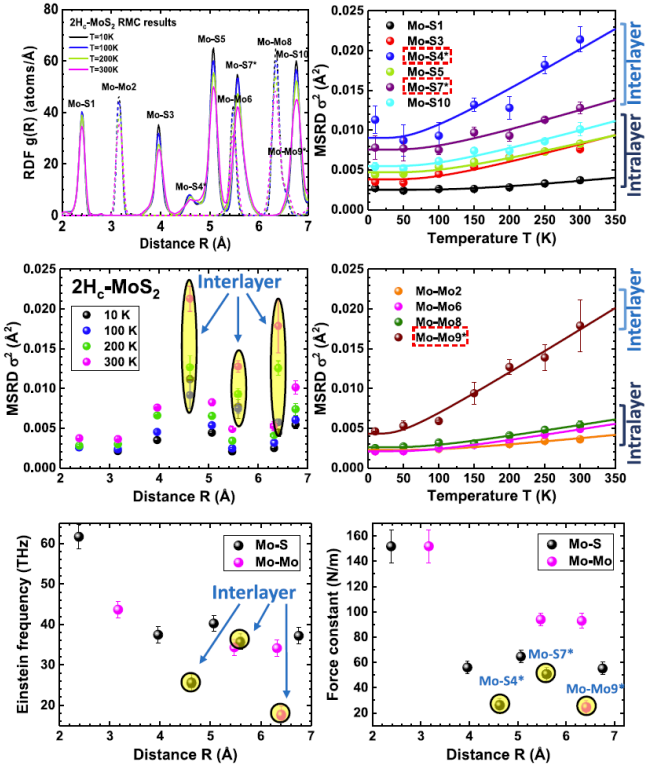
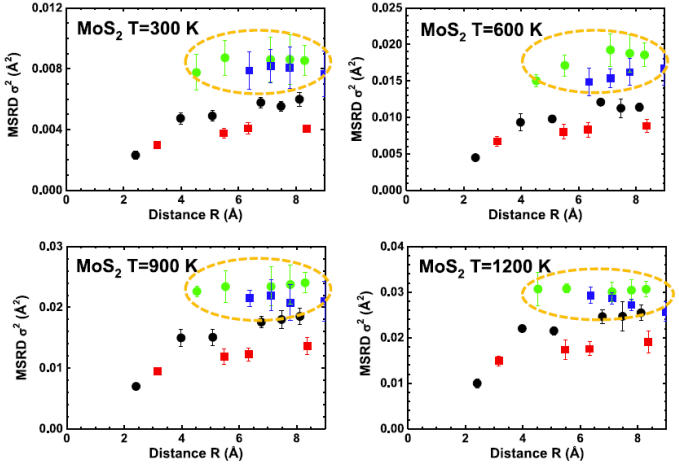


Table 1
Values of Mo–S and Mo–Mo interatomic distances for the first ten coordination shells of molybdenum calculated from the crystallographic structure of $2H_c$-MoS_2 [55]. Interlayer distances are given in bold. The values of characteristic Einstein frequencies (ω_E) and the effective force constants (κ) obtained from the RMC analysis are also given.

Atom pair	Distance (Å)	ω_E (THz)	κ (N/m)
Mo_0–S_1	2.37	62 ± 3	152 ± 13
Mo_0–Mo_2	3.16	44 ± 2	152 ± 13
Mo_0–S_3	3.95	38 ± 2	56 ± 5
Mo_0–S_4	**4.64**	**26 ± 2**	**26 ± 5**
Mo_0–S_5	5.06	40 ± 2	65 ± 5
Mo_0–Mo_6	5.48	34 ± 2	94 ± 5
Mo_0–S_7	**5.62**	**36 ± 2**	**51 ± 5**
Mo_0–Mo_8	6.32	34 ± 2	93 ± 6
Mo_0–Mo_9	**6.41**	**18 ± 2**	**25 ± 5**
Mo_0–S_{10}	6.75	37 ± 2	55 ± 5

$$\sigma^2_{\text{th}} = \langle u_A^2 \rangle + \langle u_B^2 \rangle - 2\langle u_A u_B \rangle$$

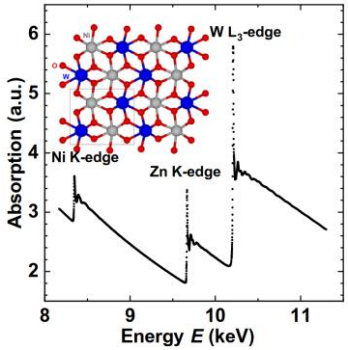
MSRD or Debye-Waller factor — MSD — MSD — Correlation



Interactions between neighbouring layers in 2D compounds can be probed by EXAFS!

I. Pudza, D. Bocharov, A. Anspoks, M. Krack, A. Kalinko, E. Welter, A. Kuzmin, Mater. Today Commun. 35 (2023) 106359.

Dimerization of nickel ions in $NiWO_4$ and $Zn_cNi_{1-c}WO_4$ solid solutions

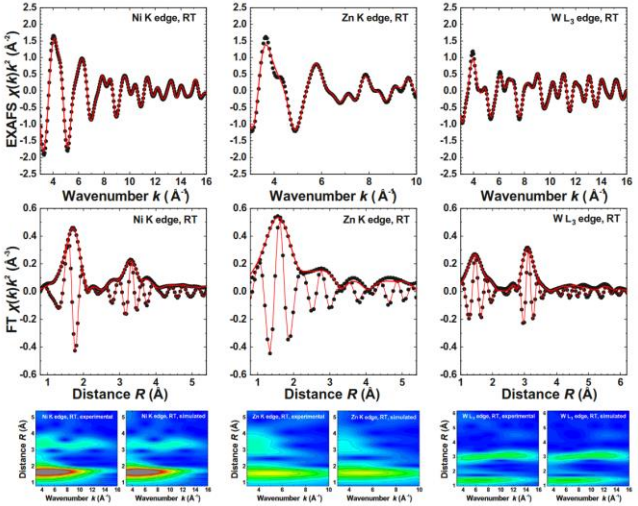


X-ray absorption spectrum of microcrystalline $Zn_{0.6}Ni_{0.4}WO_4$ spanning across the range of the Ni and Zn K-edges and W L_3-edge at 300 K.

Antiferromagnetic $NiWO_4$
$T_{Néel}$ = 60-67 K

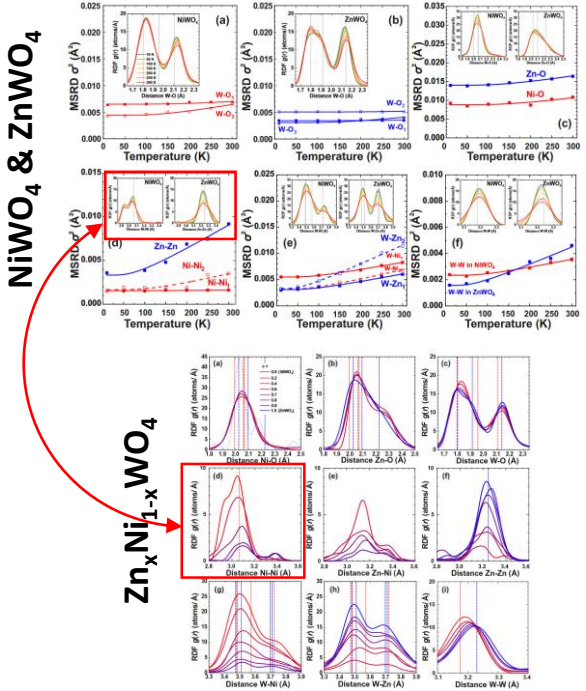
P2/c (13)
monoclinic

RMC



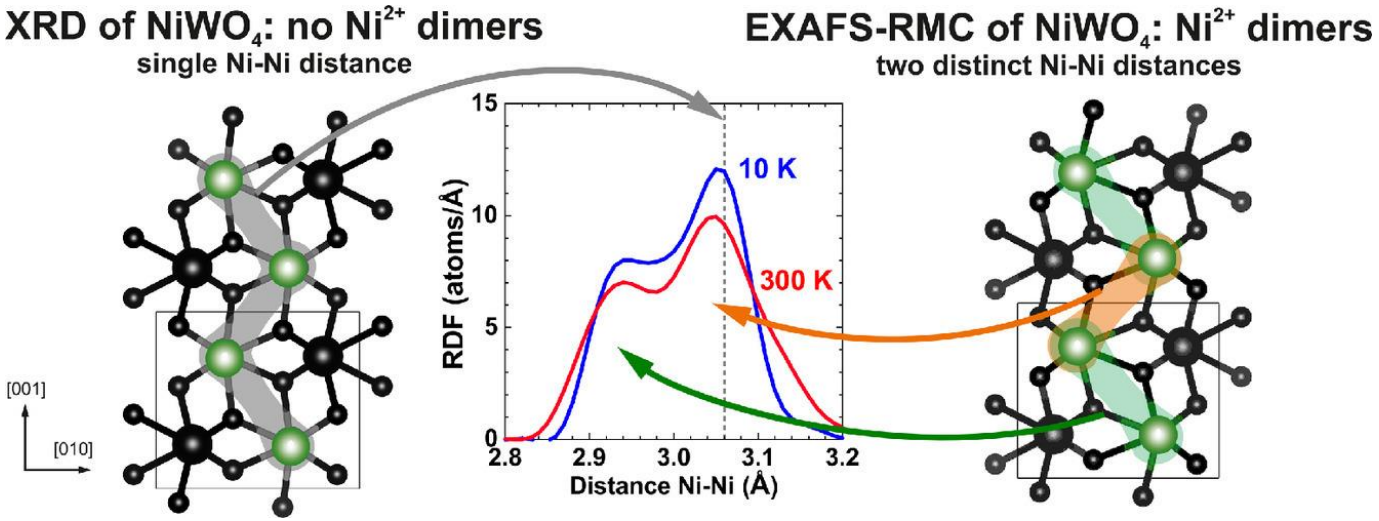
Experimental (black dots) and simulated (solid lines) extended X-ray absorption fine structure (EXAFS) spectra $\chi(k)k^2$ of $Zn_{0.6}Ni_{0.4}WO_4$ solid solution at the Ni and Zn K-edges and W L_3-edge (top row), their Fourier transforms (FTs) (middle row) and wavelet transforms (bottom row) at 300 K.

RDF



G. Bakradze, A. Kalinko, A. Kuzmin, Evidence of dimerization of nickel ions in $NiWO_4$ and $Zn_cNi_{1-c}WO_4$ solid solutions probed by EXAFS spectroscopy and reverse Monte Carlo simulations, Acta Mater. 217 (2021) 117171.

Dimerization of nickel ions in $NiWO_4$ and $Zn_cNi_{1-c}WO_4$ solid solutions



- Dimerization of Ni^{2+} ions within quasi-one-dimensional zigzag chains of $[NiO_6]$ octahedra was evidenced in $NiWO_4$ in the whole studied temperature range. It manifests itself as the splitting of the Ni–Ni radial distribution function into two separate peaks.
- The effect is further preserved in solid solutions $Zn_cNi_{1-c}WO_4$ for $c \leq 0.6$, which is related to the probability to find two Ni^{2+} ions in neighbouring positions.

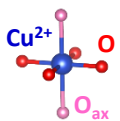
G. Bakradze, A. Kalinko, A. Kuzmin, Evidence of dimerization of nickel ions in $NiWO_4$ and $Zn_cNi_{1-c}WO_4$ solid solutions probed by EXAFS spectroscopy and reverse Monte Carlo simulations, Acta Mater. 217 (2021) 117171.

Medium- and High-Entropy Tungstates AWO_4 (A=Mn, Co, Ni, Cu, Zn)

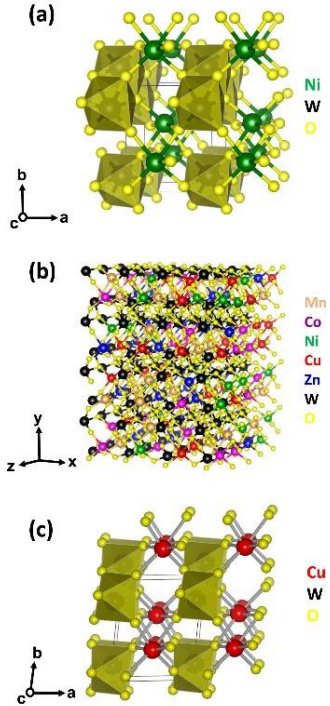
P2/c (13) monoclinic

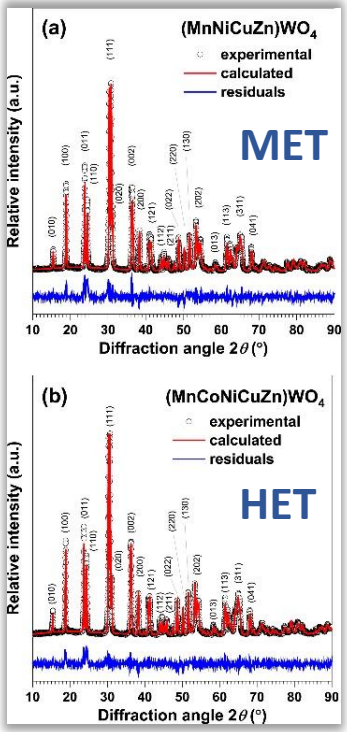
P2/c (13) monoclinic

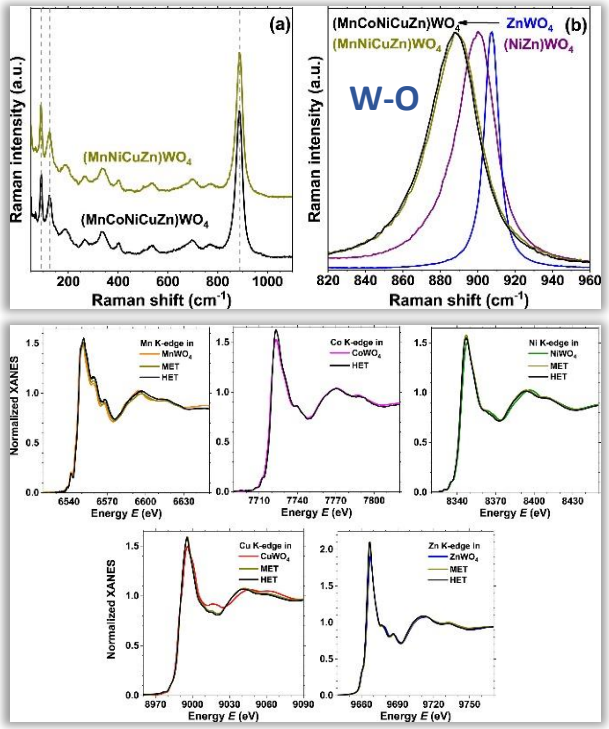
P-1 (2) triclinic



Jahn-Teller distortion

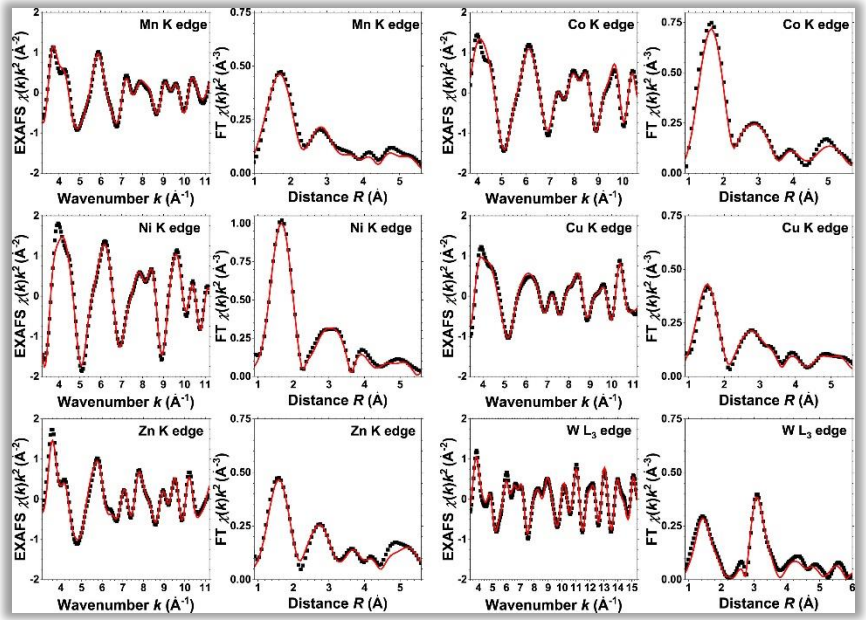






G. Bakradze, E. Welter, A. Kuzmin, Peculiarities of the local structure in new medium- and high-entropy, low-symmetry tungstates, J. Phys. Chem. Solids 172 (2023) 111052.

Medium- and High-Entropy Tungstates AWO_4 (A=Mn, Co, Ni, Cu, Zn)



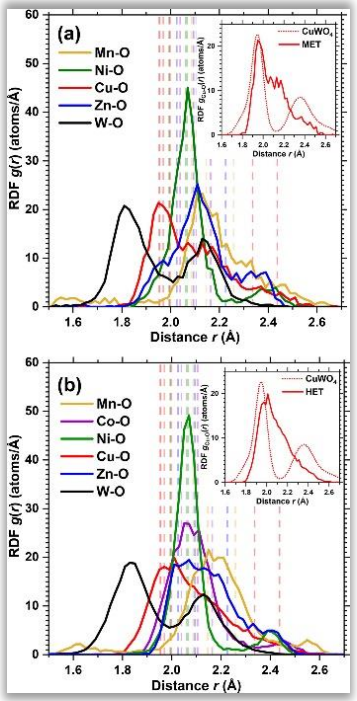


Table 1. Jahn–Teller distortion parameter, σ_{JT} (Å), for different octahedra in medium-entropy tungstate (MET) $(MnNiCuZn)WO_4$ and high-entropy tungstate (HET) $(MnCoNiCuZn)WO_4$ at 10 K.

	MET	HET
$[MnO_6]$	0.163 ± 0.092	0.152 ± 0.090
$[CoO_6]$	–	0.102 ± 0.052
$[NiO_6]$	0.091 ± 0.057	0.085 ± 0.056
$[CuO_6]$	0.140 ± 0.051	0.131 ± 0.049
$[ZnO_6]$	0.122 ± 0.046	0.115 ± 0.043
$[WO_6]$	0.159 ± 0.033	0.161 ± 0.038

Conclusions:

- Ni^{2+} ions have regular octahedral environment.
- Mn^{2+}, Co^{2+}, and Zn^{2+} ions have distorted octahedral environment.
- **$[Cu^{2+}O_6]$ octahedra are less distorted than expected for a Jahn-Teller centre.**

G. Bakradze, E. Welter, A. Kuzmin, Peculiarities of the local structure in new medium- and high-entropy, low-symmetry tungstates, J. Phys. Chem. Solids 172 (2023) 111052.

Conclusions

Advantages of the RMC method:

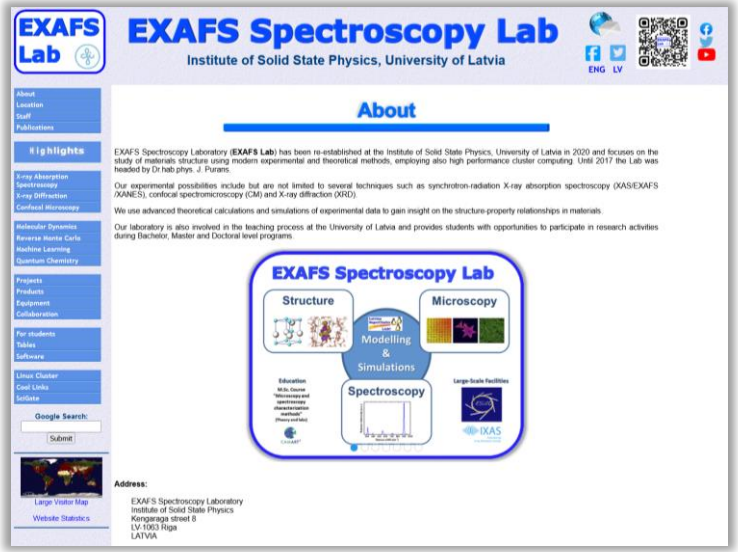
- A natural way to include disorder (static and dynamic, also anharmonic) into EXAFS simulations taking into account multiple-scattering effects.
- Reliable interpretation of EXAFS far beyond the first coordination shell is possible.
- Analysis at several absorption edges is possible in multicomponent compounds.
- Information on atom-atom and bond-angle distributions and correlations can be obtained.
- Constraints can be easily incorporated to account for information from other experiments (diffraction, total scattering, etc) or chemical/geometrical information (bond-lengths, bonding angles, coordination, energetics, etc).

Peculiarities of the RMC method:

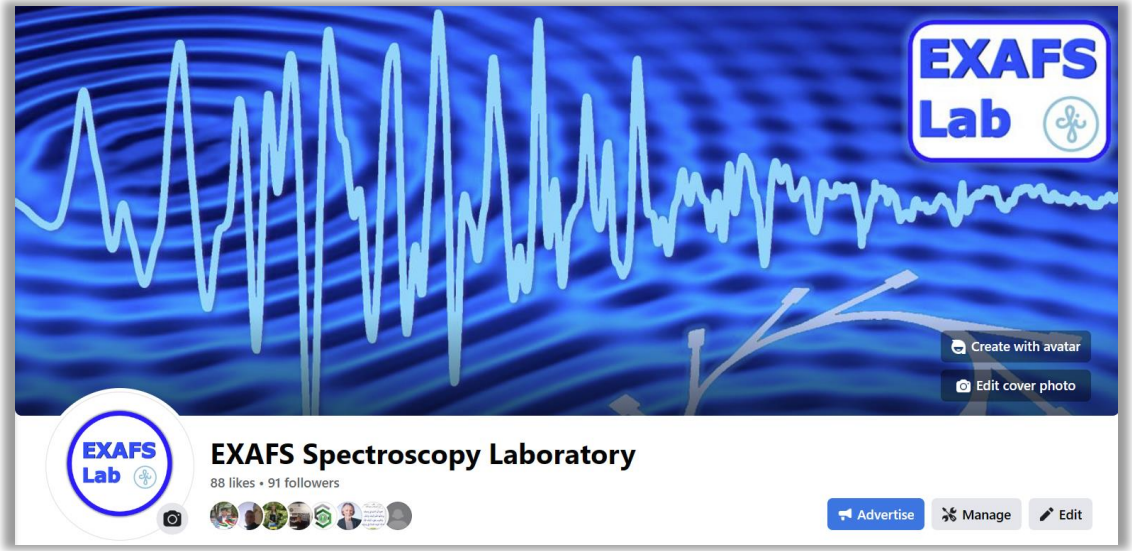
- RMC gives the most disordered solution.
- Several simulations are often required for good statistics.
- RMC is sensitive to noise.
- One should be careful with the size of the simulation box.

Thank you for your attention!

http://www.dragon.lv/exafs/

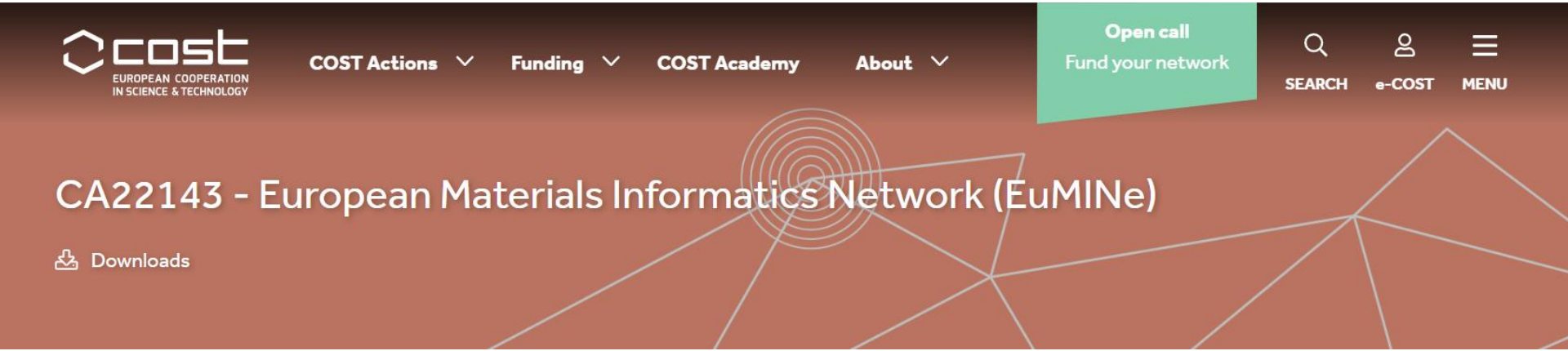


https://www.facebook.com/EXAFSLab/



FLPP
FUNDAMENTAL AND APPLIED RESEARCH PROJECTS

The work was supported by the Latvian Council of Science project No. lzp-2022/1-0608.



https://www.cost.eu/actions/CA22143/

The new COST program "European Materials Informatics Network" (EuMINe) is dedicated to the development, engineering and improvement of materials based on materials informatics, artificial intelligence (AI) and data-centric technologies.

The action period is from 24/10/2023 to 23/10/2027.