Past, Present and Future of Reverse Monte Carlo Modeling: Recent Challenges in Determining Structure- Property Relationship in Materials

861. WE-Heraeus-Seminar

27. – 31. July 2026

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 861. WE-Heraeus-Seminar:

Disordered materials, including liquids, glasses, and partially ordered solids, are central to both everyday life and advanced technologies, from battery electrodes and catalysts to phase-change memory materials. Understanding their atomic-level structure is crucial for unlocking their functional properties, such as ion conduction in battery materials or optical switching in phase-change compounds. However, unlike perfect crystals, where diffraction techniques provide direct atomic positions, disordered systems require complementary approaches to reveal structural correlations beyond the nearest-neighbor scale.

Reverse Monte Carlo (RMC) modeling has emerged as a powerful computational tool for reconstructing atomic configurations from experimental data, including X-ray and neutron scattering. By iteratively refining atomic positions to match measured structure factors, RMC provides insights into short- and intermediate-range order, structural motifs, and hidden correlations. The method has successfully been applied to liquids, covalent and metallic lasses, and disordered crystals, advancing our understanding of many complex structural henomena.

Despite its successes, challenges remain, particularly in integrating energetic constraints and overcoming the inherent under-determination of experimental data. Recent advances, including hybrid RMC approaches and AI-driven modeling, offer promising pathways to enhance structural reliability.

This seminar will bring together experts from diverse disciplines—including materials science, condensed matter physics, computational modeling, and scattering communities—to discuss state-of-the-art developments and future directions. By fostering interdisciplinary exchange between early career and experienced researchers, we aim to drive innovation in the structural analysis of disordered materials and strengthen collaborations across research fields.

We hope that individual inspirations and mutual collaborations born in this seminar offer a new avenue for a next-generation materials science.

Introduction

Scientific Organizers:

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Registration:

At the Physikzentrum, reception office
Monday (17:00 h – 21:00 h) and Tuesday morning

Program

Program

Monday, 27 July 2026

17:00 – 20:00	Registration	
18:00	*BUFFET SUPPER and informal get-together*	
19:30 – 20:30	Robert McGreevy	**The first 10 years of RMC and the next 10 years of ML' or 'The power of images'**

Tuesday, 28 July 2026

07:30	*BREAKFAST*	
08:45 - 09:00	Scientific organizers	**Welcome words**
09:00 – 09:40	Matt Tucker	**38 years of Reverse Monte Carlo Modelling**
09:40 – 10:20	Martin Dove	**Data quality and RMC**
10:20 – 10:50	*COFFEE BREAK*	
10:50 – 11:30	Mirijam Zobel	**Modulation Excitation Pair Distribution Function Experiments to Increase Phase Sensitivity**
11:30 – 11:45	Roman Holomb	**Laser-induced structural transformations in chalcogenides: finite-cluster approach to local structural rearrangements**
11:45 – 12:00	Adam Edward Stones	**Inverting PDFs to measure effective interactions decodes complexity in amorphous calcium carbonate**
12:00	*LUNCH*	

Program

Tuesday, 28 July 2026

14:00 – 14:40	Thibault Charpentier	**Designing structural disorder in oxide glasses from NMR: A Reverse Monte Carlo approach**
14:40 – 15:20	Dora Zalka	**RMC-XANES builder: A flexible workflow for XANES calculations**
15:20 – 15:50	*COFFEE BREAK / Flash poster test*	
15:50 – 17:00	**Flash poster session**	
17:00 – 18:00	**Poster session**	
18:00	*DINNER*	
19:30 – 20:30	**Poster session** (continued)	

Program

Wednesday, 29 July 2026

07:30	*BREAKFAST*	
08:45 – 09:25	Alexei Kuzmin	**From atomic structure to color switching**
09:25 – 10:05	Markus Winterer	**Combining Reverse Monte Carlo analysis of X-ray scattering and extended X-ray absorption spectroscopy**
10:05 – 10:35	*COFFEE BREAK*	
10:35 – 11:15	Ildiko Pethes	**Using EXAFS in RMC++ for amorphous materials: Features and advantages**
11:15 – 11:30	Hanna M. Wenzel	**Molecular RMC on tetrel-chalcogenid clusters with extreme nonlinear optical properties**
11:30 – 11:45	Thomas Nicholas	**The structure and topology of an amorphous metal–organic framework**
11:45 – 12:00	Valeri Petkov	**Resonant total scattering and differential PDFs in Reverse Monte Carlo modeling**
12:00	*LUNCH*	
13:30 – 18:00	**Excursion**	
18:30	*HERAEUS DINNER* *(social event with cold & warm buffet with complimentary drinks)*	

Program

Thursday, 30 July 2026

07:30	*BREAKFAST*	
08:45 – 09:25	David Keen	**Measuring total scattering data faster than the timescales of dynamical processes: implications for structural modelling**
09:25 – 10:05	Karen Appel	**Application of single shot pair distribution function techniques during shock compression at EuXFEL to study melt structure in-situ**
10:05 – 10:35	*COFFEE BREAK*	
10:35 – 11:15	Andrew Goodwin	**Understanding amorphous networks with HRMC**
11:15 – 11:30	Wojciech Slawinski	**RMC reveals hidden complexity in D_2O Ice VII**
11:30 – 11:45	Ida Nielsen	**Local structure of hydrated and dehydrated prussian white cathode materials**
11:45 – 12:00	Ying-Lung Steve Tse	**Flexible polarizable water model parameterized via gaussian process regression**
12:00	*LUNCH*	

Program

Thursday, 30 July 2026

14:00 – 14:40	Andrea Fantin	**Chemical short-range order in high-entropy alloys: Experimental limitations and implications for Reverse Monte Carlo modeling**
14:40 – 14:55	Lewis Owen	**Exploring local structure in metallic systems - challenges and opportunities**
14:55 – 15:10	Niels Schreiner	**Characterization of short range order in Ni_4Mo and its disorder-order transition through total scattering and Reverse Monte Carlo modelling.**
15:10 – 15:40	*COFFEE BRREAK*	
15:40 – 15:55	Lei Tan	**RMC Study of local structure and disorder in inorganic halide lead perovskite quantum dots**
15:55 – 16:10	Long Yang	**3D Probing of hidden nanoscale states in functional materials**
16:10 – 16:25	Akihisa Koga	**Stealthy hyperuniform bond disorder in the honeycomb Hubbard model**
16:25 – 18:00	**Poster** session	
18:00	*DINNER*	

Program

Friday, 31 July 2026

07:30	*BREAKFAST*	
08:45 – 09:25	Yohei Onodera	**Density-driven interplay of pentahedral pyramids and octahedra for high dielectric permittivity in bulk amorphous alumina**
09:25 – 09:40	Pál Jóvári	**Short-range order in $GeSb_2S_5$-Ag glasses**
09:40 – 10:20	Ayako Nakata	**Efficient analysis of local properties in complex systems by large-scale DFT and statistical methods**
10:20 – 10:50	*COFFEE BREAK*	
10:50 – 11:30	Albert Bartok-Partay	**Structure elucidation using machine learning based property predictions and interatomic potentials**
11:30 – 11:45	Yuanpeng Zhang	**Combining exhaustive symmetry and attention based learning for phase transition studies**
11:45 – 12:00	Scientific organizers	**Closing words**
12:00	*LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Saturday; however, a self-service breakfast will be provided on Saturday morning

Posters

Posters

Mohamed Ait Oufakir	**Smart solar breakthrough: Machine learning powers next-gen $CsSnI_3$/Si tandem cells**
Khadija Boughanbour	**Optimizing lead-free $FASnI_3$-based perovskite solar cells using SCAPS-1D: A numerical study with different hole transport layers (HTLs)**
Younes Chrafih	**Experimental and DFT study of Ce-doped $LaNiO_3$ perovskite for photo-assisted oxidation processes**
Gabriel Cuello	**Probing the local lithium environment in Li-rich and Mn-rich disordered rocksalt materials for battery applications: a combined neutron and X-ray pair distribution function study**
Vitalijs Dimitrijevs	**RMC-EXAFS study of local structure in WO_3 nanoparticles**
Tristan Dolling	**A mixed ligand approach to amorphisation control in zeolitic imidazolate frameworks (ZIFs)**
Joanna Grelska	**RMCProfile7: Investigation of the local structure of hydrogenated high entropy alloys**
Junbiao Guo	**Comparative study of ZrV_2O_7 and ZrP_2O_7 by lattice dynamics simulations and neutron total scattering measurements: exploring the different thermal expansivities**
Anna Herlihy	**Total scattering and RMC insights into disorder in the Bismuthinite-Aikinite series**
Satoshi Hiroi	**Crystal PDF full-space refinement: An RMCPOW-derived approach for high-precision structure analysis of crystalline materials**
Max Hirschberger	**Spin dynamics and magnetic interactions in the trimer-host compound $Dy_3Ru_4Al_{12}$**

Posters

Shinya Hosokawa	**Anomalous x-ray scattering to strengthen partial local atomic investigations in reverse Monte Carlo analyses**
Bastien Izacard	**Design of two-phase hyperuniform photonic materials for complete band gaps**
Jiri Jancalek	**Tracking the Amorphous-to-Crystalline transition in solvothermal Sb_2S_3: Evolution of short- and long-range order**
Anna Janowska	**Investigation of the molecular structure of molten metronidazole**
Sergey Kasatikov	**Investigation of the local electronic structure and chemical bonding in Pd- and Pt-based bulk metallic glasses by X-ray spectroscopy.**
Chika Kawagoe	**Local structural analysis of amorphous Ce–Mn alloys by X-ray total scattering and RMC simulation**
Julija Lukasevica	**Element-specific local distortions in the high-entropy oxide (MgCoNiCuZn)O**
Tobias Mølgaard Nielsen	**Whole-nanoparticle-ensemble refinements of compositionally complex systems from X-ray pair distribution function data via the Reverse Monte Carlo method**
Fathima Nida Pankuzhiyil Shahidrafeeque	**Barocaloric materials for solid state cooling**
Anna Piekara	**Hidden structural complexity in Ammonia Borane**
Szilvia Pothoczki	**Characterization of the solvation shell of pyranose and furanose forms of hexose molecules using classical and ab initio molecular dynamics**

Posters

Johannes Spiegel	**Intermetallic phases and liquid alloys in Pt-Ga SCALMS by pair distribution function analysis**
Chloe Sutre	**Probing the local lithium environment in Li-rich and Mn-rich disordered rocksalt materials for battery applications: a combined neutron and X-ray pair distribution function study**
Nayuta Takemori	**From structure to function in aperiodic systems: Photonic band gaps in quasiperiodic tilings**
Laszlo Temleitner	**How does high pressure alter the hydrogen-bonded network in liquid methanol-water mixtures?**
Jan Hendrik Thimm	**Molecular RMC modeling on combined data sets and a showcase of XRD software package A_2D_2**
Gergely Tóth	**Pair potential from force distribution and corresponding configurations**
Benjamin Tragheim	**Resolving local structural influences in quasi-linear dielectric, $NaNbO_3$-based systems using total scattering techniques**
Kazuki Yoshikawa	**Water hydration at high pressure in Cu^{2+} solutions probed by x-ray absorption fine structure**
Daria Zandberg	**Probing ZnO lattice dynamics via EXAFS and reverse Monte Carlo modeling**
Simone Ziglio	**Temperature-dependent structural evolution in glassy GeO2: a Reverse Monte Carlo study**

Abstracts of Talks

(in alphabetical order)

Application of single shot pair distribution function techniques during shock compression at EuXFEL to study melt structure in-situ

K. Appel[1] et al.

[1]European XFEL, Schenefeld, Germany

With the opening of hard X-ray Free Electron Laser facilities (XFEL), single shot total scattering data of short-lived systems have become potentially accessible for pump-probe experiments. One possible new application is optical laser induced shock compression of materials to study melt structures at extreme temperatures and pressures.

The High-Energy Density Helmholtz International Beamline of Extreme Fields (HED-HIBEF) at European XFEL provides a 100 J class long pulse laser (DiPOLE100-X) that can be coupled to X-rays produced by the process of self-amplified spontaneous emission at the SASE2 undulator source of HED-HIBEF in the range of 5 – 25 keV [1]. The capability of studying material at extreme conditions by pair distribution function (PDF) techniques has been exploited from the first user experiment with DiPOLE100-X onwards [2,3]. The optimization of the experimental set-up and data analysis chain for PDF techniques is subject of the only long-time proposal (LTP, led by D. Keen) at the beamline [4].

In this talk, I will present results on experimental data taken on shock compressed liquid tin [2], carbon [3], Fe oxides [5] and silica with the standard X-ray diffraction set-up at interaction chamber 2 of HED-HIBEF which demonstrate that the determination of the liquid structure is feasible in simple and complex liquids by single shot pump-probe experiments at HED-HIBEF. In addition, I will discuss the potential of a new detector arrangement as realized during the LTP in interaction chamber 1 of the HED-HIBEF beamline [4]. In the last part, I will show an overview of the data analysis workflow which was developed for the EuXFEL single shot data and give an outlook on future plans to optimize the PDF technique at HED-HIBEF.

We acknowledge EuXFEL for providing beamtime in two standard proposals (#2740 and #6746), a HIBEF Priority Access Proposal (#6659) and a long-term proposal with two beamtimes so far at HED-HIBEF (#3248 and # 7316).

References

[1] U. Zastrau, Journal of Synchrotron Radiation **28**, 1393 (2021)
[2] M. Gorman, Journal of Applied Physics **135**, 165902 (2024)
[3] D. Kraus, Nature **642**, 351 (2025)
[4] A. Sapnik, IUCrJ **12**, 531 (2025)
[5] C. Crépisson, arXiv preprint arXiv:2511.20144 (2025)

Structure elucidation using machine learning based property predictions and interatomic potentials

A. Bartók-Pártay[1,2]

[1]Department of Physics, University of Warwick, Coventry, United Kingdom
[2] Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, United Kingdom

Ab initio electronic structure calculations hold the promise to predict and explain material properties, based on atomic scale simulations. While accurate and predictive, ab initio methods are often limited by unfavourable scaling with system size and generally, their great computational expense, preventing them from reaching many relevant time- and length-scales. In the past two decades, machine learning (ML) techniques were adapted as surrogate models for electronic structure calculations, retaining the accuracy of ab initio calculations while achieving multiple orders of magnitude speed-ups. Modest amounts of data obtained from electronic structure calculations can be used to train ML models, to be used in production simulations of matter, in significantly larger system sizes and allowing more exhaustive sampling than previously possible.In this talk, I will discuss the theory of atomistic ML, highlighting recent advances and remaining challenges. I will show our results on modelling amorphous silicon using a machine learned interatomic potential: generating realistic structures from melt-quench simulations and validating these against experimental diffraction and solid-state NMR data[1]. While molecular dynamics, especially when combined with a fast and accurate interatomic potential, is a powerful tool to sample atomic structures, accessing thermodynamically metastable states remains a challenge. For example, time-scales in experimental preparation of disordered materials may still be out of reach even with ML-assisted speed-ups, or it may be impractical to replicate all aspects of the experimental procedure. For example, oxygen-rich amorphous carbon materials are prepared by deposition, a non-equilibrium process that strongly influences the resulting microscopic structure[2]. To access these structures, we carried out a Monte Carlo simulation study, where we applied both a machine-learned interatomic potential and a machine-learned model of core electron binding energies. Using the latter, the X-ray photoelectron spectrum can be predicted, and used to guide the simulation towards experimentally observed spectra. Sampling this combined landscape resulted in high quality structural models that can be used in the design and interpretation of amorphous carbon materials.

References

[1] V.L. Deringer et al, J. Phys. Chem. Lett. **9**, 2879 (2018)
[2] T. Zarrouk, R. Ibragimova, A. P. Bartók, and M. A. Caro, J. Am. Chem. Soc. **146**, 14645 (2024).

Designing Disorder in Oxide Glasses from NMR : a Reverse Monte Carlo Approach

Thibault Charpentier

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Solid-state NMR has clearly establish itself as an essential spectroscopy technique for studying oxide glasses, as it offers a wide range of techniques for studying both their structure and dynamics at an atomic scale. However, the information obtained is limited to short-range order (elementary structural motifs constituting the glass network) and medium-range order (connectivity or proximity between these motifs). However, alone, it does not allow three-dimensional structural models to be constructed. To this end, Molecular Dynamics (MD) is therefore crucial for generating three-dimensional atomic structures of a glass at a larger length scale. Thanks to DFT-NMR calculations, structural models developed by MD can be directly connected to NMR spectra, [1] which can greatly facilitate the interpretation of experimental data. However, topology of such models are inherently limited by the accuracy of MD force-fields and/or the accessible time-scale to MD.

Reverse Monte Carlo [2] modeling provides a very efficient approach to overcome these limitations because it can generate structural models (by random atomic displacements) that reproduce available experimental data (generally neutron and X-ray structure factors). We will show how NMR information characterizing short- and medium-range order can be integrated into these simulations to produce glassy structures that cannot be produced by molecular dynamics. In the current context of increasingly frequent use of machine learning, these simulations also offer the possibility of producing structures with predefined patterns to effectively build libraries of NMR spectral signatures. This is crucial for the development of databases offering a sufficient structural diversity for the development of transferable ML force fields for example. We will illustrate these advances in the development of NMR-driven structural modelling for different oxide glasses, and its combination with equivariant Machine Learning (ML) for the prediction of NMR interactions. [3]

[1] T. Charpentier, M.C. Menziani, A. Pedone, RSC Adv. 3, 10550-10578 (**2013**);
[2] R.L McGreevy, P Zetterström, J. of Non-Cryst. Solids 293–295, 297-303 (**2001**)
[3] Z. Chaker, M. Salanne, J.-M. Delaye, T. Charpentier Phys Chem Chem Phys. 21, 21709-21725 (**2019**) ; T. Charpentier, Faraday Discuss., 255, 370-390 (**2025**)

Data Quality and RMC

Martin T Dove

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And Queen Mary University of London, London, UK

The quality of an RMC simulation depends critically on the quality of the data to be used. There are some issues about data quality that have tended to be ignored to some extent. These include the neglect of instrument resolution, which will be different for different banks of detectors for measurements with spallation neutron sources, and inadequate treatment of approximately-additive corrections to the data (such as for inelasticity or Comptron scattering). Inadequacies of these corrections may be hidden with a single detector (as in X-ray scattering), but for neutron scattering at a spallation source, it is clear that even in the best cases, the data for different detectors never align, often by a significant degree. Even worse is my feeling that data quality today is declining; I see many papers where the PDFs clearly suffer from deficiencies, particularly at low distances.

We have been working on new methods to extract the PDF from total scattering data so that we can account for resolution functions and for additive errors in both the merged scattering functions and the resultant PDF [1]. To deal with the additive errors we have adapted a method developed by Billinge and Farrow [2], and to deal with the resolution we exploit the possibility to represent the scattering functions and PDF in terms of Hermite functions. We show how total scattering data and the PDF generated by this method has been used in a study of disorder associated with the phase transition in copper pyrophosphate, $Cu_2P_2O_7$ [3].

References

[1] S Wang, M Gao, Y Qin, S Zhang, L Tan and MT Dove. Accounting for instrument resolution in the pair distribution functions obtained from total scattering data using Hermite functions. *J. Appl. Cryst.* **58**, 1269–1287, 2025 (10.1107/S1600576725004340)

[2] SJL Billinge and CL Farrow. Towards a robust ad hoc data correction approach that yields reliable atomic pair distribution functions from powder diffraction data. *J. Phys. Condens. Matter* **25**, 454202,2013 (10.1088/0953-8984/25/45/454202)

[3] MT Dove, N Shi, S Wang, J Song, J Xu, W Yin, J Chen, H Yang and G Cai. Phase transition and negative thermal expansion in copper pyrophosphate $Cu_2P_2O_7$ studied by neutron total scattering and the reverse Monte Carlo method. *Phys. Rev. B*, in press, 2026

Chemical short-range order in High-Entropy Alloys: experimental limitations and implications for Reverse Monte Carlo modeling

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Understanding the complex atomic-scale structures within High-Entropy Alloys (HEAs) is crucial for tailoring their properties to diverse applications. The present contribution provides an overview of state-of-the-art experimental techniques employed to probe local lattice distortions and chemical short-range order in HEAs, ranging from synchrotron- and neutron-based methods such as X-ray absorption spectroscopy and total scattering to emerging approaches including single-crystal diffuse scattering and atomic-resolution holography.

A primary challenge in multicomponent alloys lies in the inherently reduced scattering contrast between constituent elements, which are often neighbors in the periodic table and occupy simple crystal structures with few crystallographic sites. This limitation constrains the amount of structural information that can be extracted from experimental data, a challenge that also extends to high-resolution transmission electron microscopy. At the laboratory scale, complementary thermophysical techniques such as differential scanning calorimetry and electrical resistivity have proven valuable for corroborating and quantifying ordering phenomena. It becomes evident that no single experimental technique is sufficient to fully resolve the structural complexity of HEAs. Instead, a combination of complementary methods, ideally supported by simulations, is required to disentangle the contributions of different atomic species and relate local structure to macroscopic properties. At the same time, it is important to recognize that the information content of any structural model—including those obtained via Reverse Monte Carlo (RMC)—remains fundamentally constrained by the sensitivity and contrast of the underlying experimental data.

In this context, the application of RMC to multicomponent alloys highlights both its strengths and its intrinsic challenges. When scattering contrast between elements is low, structural solutions may suffer from non-uniqueness and reduced chemical specificity. This observation motivates the integration of RMC with physically informed constraints, such as those derived from molecular dynamics or Monte Carlo simulations, in order to incorporate energetic considerations alongside data fitting. Such hybrid approaches represent a promising pathway toward more realistic and predictive structural models, ultimately improving our ability to establish robust structure–property relationships in complex alloys.

[1] A. Fantin et al., *Acta Materialia* 193, 329–337 (2020)
[2] A. Fantin et al., *Materials Research Letters* 12(5), 346–354 (2024)
[3] V. Bacurau et al., *Nature Communications* 15, 7815 (2024)

Understanding amorphous networks with HRMC

A. L. Goodwin

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Hybrid reverse Monte Carlo (HRMC) methodologies use energy calculations to bias the configurational landscape explored during RMC refinement [1]. Whereas HRMC methods historically employed relatively simple harmonic potentials, it is now possible to use high-quality complex empirical potentials and even machine-learned interatomic potentials to carry out HRMC refinements [2]. This talk will focus on two recent applications within our own group: the determination of structural models of amorphous calcium carbonate [3] and an amorphous zeolitic imidazolate framework [4]. A particular emphasis will be on the effect of increasing complexity of energetic calculations involved on the scientific conclusions drawn in each case [5,6].

References

[1] G. Opletal, T. Petersen, B. O'Malley, I. Snook, D. G. McCulloch, N. A. Marks & I. Yarovsky, *Mol. Simul.* **28**, 927 (2002).
[2] P. Cuillier, M. G. Tucker & Y. Zhang, *J. Appl. Cryst.* **57**, 1780 (2024).
[3] T. C. Nicholas, A. E. Stones, A. Patel, F. M. Michel, R. J. Reeder, D. G. A. L. Aarts, V. L. Deringer & A. L. Goodwin, *Nat. Chem.* **16**, 36 (2024).
[4] T. C. Nicholas, D. F. T. du Toit, L. A. M. Rosset, D. M. Proserpio, A. L. Goodwin & V. L. Deringer, *arXiv*:2503.24367 (2025).
[5] A. L. Goodwin, F. M. Michel, B. L. Phillips, D. A. Keen, M. T. Dove & R. J. Reeder, *Chem. Mater.* **22**, 3197 (2010).
[6] T. D. Bennett, A. L. Goodwin, M. T. Dove, D. A. Keen, M. G. Tucker, E. R. Barney, A. K. Soper, E. G. Bithell, J.-C. Tan & A. K. Cheetham, *Phys. Rev. Lett.* **104**, 115503 (2010).

Laser-induced structural transformations in chalcogenides: finite-cluster approach to local structural rearrangements

R. Holomb[1,2], V. Mitsa[2], O. Kondrat[2], O. Mitsa[2], L. Himics[1] and M. Veres[1]

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Amorphous and crystalline chalcogenides are important materials for infrared photonics and reconfigurable optical media because of their strong structure-property correlations and pronounced photoinduced structural response [1,2]. Their electronic and optical properties are governed by the local atomic structure, making structural control essential. Amorphous Se and As-S systems serve as model platforms for investigating disorder-induced structural transformations.

We report on the laser-induced structural transformations in Se and As-S systems studied by Raman spectroscopy, molecular modelling, and *ab initio* calculations within a finite-cluster approach, providing atomistic insight into local disorder and bonding rearrangements, and complementing large-scale Reverse Monte Carlo modelling. In Se thin films, irreversible photo-crystallization proceeds through bond breaking in Se rings, chain formation, and rearrangement into ordered helix-like trigonal Se segments. Investigations of As-S glasses and thin films reveal that cage-like As_4S_4 clusters play a key role in the laser-induced transformations. *In situ* synchrotron photoelectron spectroscopy shows that the realgar-pararealgar transformation is accompanied by near-surface As enrichment and is reversible during annealing-laser irradiation cycles [3]. Gold-nanoparticle-assisted growth was further used to synthesize As-S crystallites with cage-like structures. Uzonite-like As_4S_5 crystallites are resistant to laser-induced transformations, whereas realgar-like As_4S_4 crystallites exhibit bond rearrangements. Changes in the low-frequency Raman spectra during the laser-induced transformation indicate a direct relationship between structural disorder and Boson peak formation. These results demonstrate complementary pathways for controlling local structure and reversible transformations in chalcogenide systems and highlight the importance of finite-cluster modelling for understanding disorder-driven structural dynamics.

References

[1] R. Holomb, O. Kondrat, V. Mitsa *et al.*, J. Alloys Compd. **894**, 162467 (2022)
[2] D. Tsiulyanu, M. Veres, R. Holomb, M. Ciobanu, J. Non-Cryst. Sol. **609**, 122255 (2023)
[3] R. Holomb, O. Kondrat, V. Mitsa, M. Veres *et al.*, J. Chem. Phys. **149**, 214702 (2018)

Short-range order in $GeSb_2S_5$-Ag glasses

D. Zalka[1], M. Fraenkl[2], T. Wágner[2,3], S. Michalik[4], L. Pusztai[5], T. Honda[6] and P. Jóvári[5]

[1]European Synchrotron Radiation Facility (ESRF), Grenoble, France
[2] Department of General and Inorganic Chemistry, University of Pardubice, Pardubice, Czech Republic
[3] Center of Materials and Nanotechnologies, University of Pardubice, Pardubice, Czech Republic
[4]Diamond Light Source, Didcot, UK
[5]Wigner Research Centre for Physics, Budapest, Hungary
[6]Institute of Materials Structure Science, Neutron Science Division, Ibaraki, Japan

Ag-doped $GeSb_2S_5$ glasses exhibit an interesting combination of physical properties: Upon adding Ag DC conductivity increases several orders of magnitude, the glass transition temperature decreases and the glasses become harder [1]. The present study aims at the structural background of the above changes. The short-range order of $GeSb_2S_5$-Ag glasses is investigated by means of neutron diffraction, X-ray diffraction and extended X-ray absorption fine structure spectroscopy (EXAFS). Large scale structural models are obtained by fitting multiple datasets by the reverse Monte Carlo simulation technique (RMC). The reliability of the structural parameters obtained from RMC models is discussed in detail along with the information content of EXAFS spectra and diffraction structure factors.

References

[1] M. Fraenkl, B. Frumarova, V. Podzemna, S. Slang, L. Benes, M. Vlcek, T. Wagner, J. Non-Cryst. Solids **499**, 412 (2018)

Measuring total scattering data faster than the timescales of dynamical processes: implications for structural modelling

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Typical measurement times for total scattering are slow. Data need to be collected on the order of hours and minutes at neutron and synchrotron X-ray sources, respectively, to provide the statistical accuracy for reliable Fourier transform to the pair distribution function (PDF). This compromises the fundamental nature of total scattering that, by measuring the scattering over all energy transfers within the sample, would give an instantaneous structural description of the material if the data could be measured quickly enough.

X-ray free-electron lasers (XFELs) provide very intense pulses of X-rays with pulse widths ~25fs, far shorter than timescales associated with (for example) phonons and structural changes caused by coupling to charge and spin dynamics. However, until recently their X-ray energy was typically only sufficient to provide very low-resolution PDFs and their use for total scattering was largely limited to studies of simple liquids. This is no longer the case and this talk will describe our efforts [1] to establish high-quality total scattering measurements at the European XFEL in Hamburg. I will also to initiate a discussion about how such data might be combined with structural modelling to understand, not only the structure of disordered materials, but also the dynamics of their disordering processes.

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Stealthy hyperuniform bond disorder in the honeycomb Hubbard model

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Hyperuniform structures, characterized by the anomalous suppression of large-scale density fluctuations, have attracted growing attention as a new class of correlated disordered systems [1,2]. While their potential for controlling wave propagation has been explored in photonic and phononic systems, their impact on correlated electrons and magnetic ordering remains largely unclear.

In this study, we investigate the effects of stealthy hyperuniform bond distributions on the electronic and magnetic properties of the Hubbard model on the honeycomb lattice. The bond distributions are generated using a reverse Monte Carlo method so as to realize stealthy hyperuniform correlations with controlled structural features. By diagonalizing the noninteracting Hamiltonian, we show that a linear density of states (DOS), characteristic of the honeycomb lattice, robustly emerges even in the presence of hyperuniform bond modulations. On the other hand, the stealth property of the bond distribution makes wave functions in the higher-energy region more extended and significantly modifies the DOS near the band edge. To clarify the impact on magnetism, we apply the real-space Hartree approximation to the Hubbard model. We find that the phase transition always occurs between semimetallic and antiferromagnetically ordered states, while the critical interaction strength is sensitive to the stealth property. A comparison with the quasiperiodic honeycomb tiling further highlights the role of structural correlations. These results demonstrate that stealthy hyperuniform disorder provides a novel route to controlling electronic states and magnetic phase transitions in correlated systems [3].

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From Atomic Structure to Color Switching

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X-ray absorption spectroscopy (XAS) is a local structural tool offering unique opportunities for understanding structure-property relationships in chromogenic materials, which reversibly change their optical properties (color) in response to external stimuli, including light, heat, electric fields, gas exposure, and others. XAS provides information about the oxidation state and local environment of a specific element, as well as their variations during the color change. To extract this information reliably, analysis of the extended X-ray absorption fine structure (EXAFS) using advanced atomistic modeling techniques, such as reverse Monte Carlo simulation [1], is often preferable.

In this study, the RMC-EXAFS method was applied to explore distortions of the local atomic structure in protonated scheelite-type tungstates AWO_4 (A = Ca, Sr, Ba) [2] and photochromic yttrium oxyhydride (YHO) [3,4]. The obtained results were supported by first-principles calculations. The intercalation of H+ into the crystal structure of the tungstate results in the reduction of W(6+) to W(5+), i.e., the formation of polaronic centers responsible for the characteristic dark blue-purple color. The relaxation of the local atomic structure around the W(5+) polaronic centers was determined and suggests a displacement of the W(5+) ions from the center of the [WO_4] tetrahedra, in agreement with predictions from first-principles calculations.

A definitive understanding of the photochromic mechanism in YHO has remained elusive despite more than a decade of dedicated research. Using RMC-EXAFS analysis [3,4], splitting of the second coordination shell of yttrium ions, having an effective oxidation state of +2.5, was discovered in both the transparent and photodarkened states of YHO. The origin of this splitting was attributed to anisotropic local coordination of yttrium, in which anion vacancies are responsible for light absorption, according to first-principles calculations [4].

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‘The first 10 years of RMC and the next 10 years of ML’ or ‘The Power of Images’

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We are all now well aware of the fake images produced by AI that flood the internet, and the corrosive effect they are having on the concept of truth. But since the late 19th and early 20th century, when we moved beyond what could be seen with optical microscopes, scienctists have been producing images/models that attempt to explain ‘what lies beneath’, even when we are explaining something that we say cannot be visualised such as quantum behaviour. This works because we (although not always) understand that these images/models are *not* the truth, they are just ways of helping us to better understand the world – until new information comes along and we have to make a new image/model.

In the early years of RMC it was necessary to constantly repeat this philosophy. RMC models were never claimed to be ‘the truth’. But for a wide variety of systems they were able to help with understanding, and to make hypotheses that could be further tested. In this seminar I will highlight a few ‘favourite’ examples from the first 10 years of RMC.

Machine learning techniques are already revolutionising the collection and analysis/interpretation of scientific data. These are intrinsically methods for making models, and then predictions based on those models. And of course ML is much more powerful than MC so it seems inevitable that RMC, and similar methods, will be replaced. The expectation will increasingly be that the outcome of experiments is an image/model, and this may be obtained through hybrid methods. This is well illustrated by techniques used in cryo-electron microscopy, where the final ‘image’ is quite different from the initial ‘image’. But we will keep needing to remember that neither of them are ‘the truth’.

Efficient analysis of local properties in complex systems by large-scale DFT and statistical methods

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First-principles density functional theory (DFT) calculations are a powerful tool for investigating the correlations between atomic and electronic structures that give rise to material properties. To appropriately describe complex nanoscale structures, such as interfaces, defect complexes, and disordered systems, structural models comprising several thousand atoms or more are often required. However, the applications of conventional DFT calculations are typically limited for the systems with fewer than a thousand atoms, because the computational cost scales cubically with the number of atoms. To overcome this limitation, we have developed a large-scale DFT code CONQUEST [1]. CONQUEST handles large systems by using local orbital support functions to express density matrices and large-scale calculation techniques such as multi-site support function method [2]. Together with recent rapid advances in machine learning (ML)-based molecular dynamics (MD), it has become possible to analyze long-time dynamics of structures and electronic states of large systems.

In this presentation, we first briefly introduce our code and then discuss its recent application to metallic nanoparticles. Controlling the size of platinum nanoparticle (Pt NP) catalysts is a critical challenge in fuel-cell development. In this study, we investigate the size and site dependencies of atomic and electronic structures in Pt NPs spanning a few nanometers in diameter, which is comparable to particle sizes in practical applications. We also examine the size and site dependence of oxidation properties regarding the adsorption of O, OH, and H2O. To efficiently analyze the substantial data calculated for large systems, we have proposed a method for quantitatively and systematically comparing differences in local electronic structures via statistical analysis [3]. Energy density analysis [4] has also been recently implemented in CONQUEST. By employing these analytical methods, we investigate the relationship between local electronic and energetic properties in large and complex systems. Furthermore, we will explore the effects of temperature and H2O solvent using first-principles MD simulations in conjunction with MD based on machine-learning potentials.

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The structure and topology of an amorphous metal–organic framework

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Amorphous metal–organic frameworks combine the chemical versatility of MOFs with the attractive physical properties of the amorphous state, but their structures remain difficult to determine [1]. Existing models are often built by analogy to crystalline polymorphs or inorganic glasses, while the validity of these analogies is hard to test: total-scattering data are intrinsically underdetermined, and *in silico* approaches can struggle to access the relevant amorphous configurational landscape.

Here, we determine the structure of an amorphous zeolitic imidazolate framework, a-ZIF, by combining X-ray and neutron total-scattering data with active machine learning for interatomic potentials [2]. In this approach, scattering data guide structural exploration, while machine-learned potentials provide energetic constraints that distinguish between plausible models [3]. Embedding these potentials within hybrid reverse Monte Carlo enables access to configurations beyond conventional molecular dynamics and improves the potential through active learning. The resulting models reproduce experiment while remaining chemically realistic, revealing that a-ZIF is not topologically equivalent to amorphous silica or other tetrahedral inorganic networks. This work shows how hybrid RMC and active machine learning can overcome the information poverty of total scattering in amorphous framework materials.

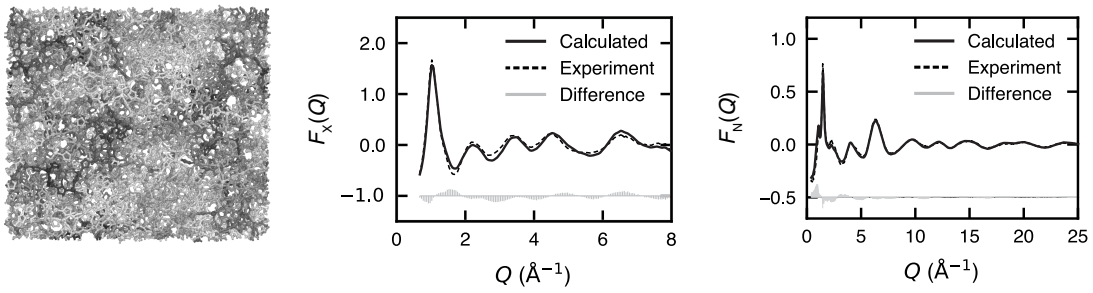

Figure 1. Data-driven model of a-ZIF. A structural model is shown alongside fits to the experimental X-ray and neutron total-scattering functions, demonstrating agreement with experiment and revealing the distinct topology of the amorphous MOF.

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Local structure of hydrated and dehydrated Prussian white cathode materials

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Prussian blue analogues (PBAs) are growing as cathode materials in sodium-ion batteries. Of particular interest is Prussian white (PW), an iron-based, vacancy-free compound with the chemical formula $Na_2Fe[Fe(CN)_6]\cdot 2H_2O$. The presence of water in PW has an opposing role in its electrochemical performance. Water helps stabilize the structure by preventing large volume changes during sodium extraction and insertion, thereby enhancing the lifetime of the material by preventing cracking. However, water in non-aqueous battery systems can lead to unwanted side reactions with the organic electrolyte. Therefore, water must be replaced with another small molecule for PW to reach its full potential in non-aqueous batteries. In addition, the position of sodium and water in PW has been debated extensively, and experimental and theoretical studies do not agree. To unravel the position of sodium and water within the PBA framework and successfully modify existing materials, a fundamental understanding of water's position and dynamics in the structure of PW as a function of temperature is necessary. Insight into the local structure of PW was obtained via neutron total scattering and inelastic neutron scattering. Reverse Monte Carlo analysis of the neutron total scattering data revealed distortions of the nitrogen-bound iron octahedra in the PBA framework. The sodium ordering in the hydrated material was found to affect the orientation of the water molecules. In the low temperature $P2_1/n$ phase, sodium orders into a plane together with the oxygen atoms, while the hydrogen atoms point away from this plane. In the room temperature $R\bar{3}$ phase, the sodium and water are more disordered despite similar frameworks. Interestingly, sodium can take a wide range of positions, spanning from the center and out to the window positions within the framework. Upon dehydration, the material becomes strained from a combination of octahedral distortions and a disordered distribution of sodium throughout the PBA framework. Thus, the position of sodium highly depends on electrostatic interactions with the cyanide (which increases with dehydration) and whether a water molecule blocks its pathway or not. This was also confirmed by inelastic neutron scattering combined with theoretical density functional theory calculations, probing only the local environment of water. Thus, there exists a co-dependent relationship between sodium and water. These results highlight the highly complex and dynamic nature of PBAs. A similar complex relationship could exist between sodium and another guest molecule, meaning that the local structure of solvent-modified PBAs must be considered to fully understand the ion transport in these materials.

Density-driven interplay of pentahedral pyramids and octahedra for high dielectric permittivity in bulk amorphous alumina

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The synthesis of single-component oxide glasses, such as Al_2O_3 (alumina), remains largely unexplored due to their lack intrinsic glass-forming ability [1]. In this study, a transparent bulk amorphous alumina with excellent thermal conductivity, hardness, and dielectric permittivity was synthesized via high pressure treatment of an amorphous porous alumina thin film. A three-dimensional atomistic model of the bulk amorphous alumina was constructed using combined reverse Monte Calor–classical molecular dynamics modelling on the basis of high-energy X-ray diffraction, neutron diffraction, and NMR data. The results reveal that fivefold-coordinated pyramidal units (AlO_5), resembling a distorted octahedron missing one oxygen vertex, serve as the primary structural motifs in amorphous alumina [2]. High-pressure treatment promotes the formation of an edge-sharing matrix composed of further distorted AlO_5 pyramids along with an increased fraction of AlO_6 octahedra, leading to enhanced dielectric permittivity exceeding that of crystalline α-Al_2O_3.

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Exploring local structure in metallic systems - challenges and opportunities

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Local structure in alloys, particularly chemical short-range order (SRO) and local lattice distortions (LLDs), has been an outstanding question in the field since the 1950s [1]. It has been suggested that these local effects may influence key physical properties of metallic systems such as strength, electrical resistivity and magnetic nature. Recently with the advent of the high-entropy alloy (HEA) or multi-principal element alloys, there has been renewed interest in understanding these effects, as many of their beneficial properties are often linked to these local environments.

In this talk, I will describe the methodologies we have developed for assessing and characterising short-range order [2,3] and local lattice distortion in metallic systems [4,5] using total scattering and RMC methods. I will discuss common errors that can lead to spurious results if not assessed correctly, and the creation of 'artificial ordering' or chemical clustering within a system [3,6]. In turn, I will discuss refinement strategies that aid in the mitigation of these effects and the extraction of the order within the system. The framework and numerical quantifiers we have developed to aid in the description and characterisation of the order present will also be presented [2,7]. Finally, we will discuss how these methods may be generalised and used in other chemical systems where local-ordering may be affecting the properties [8], including compositionally complex materials, nanoparticles and functional materials.

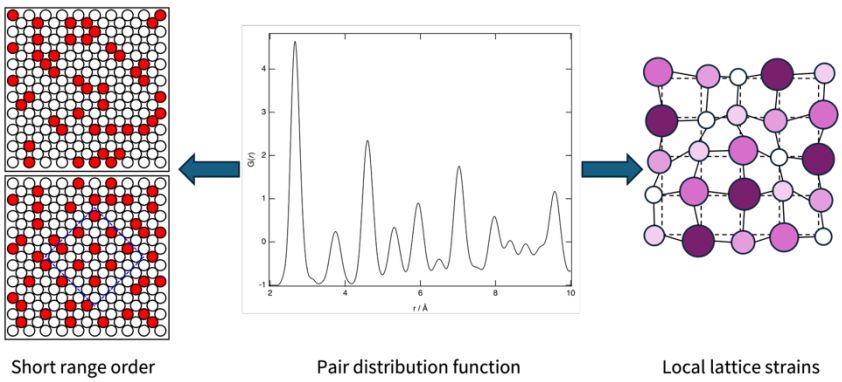

Figure 1 – Schematic illustration of a PDF and the most common local structural effects in a metallic system

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Using EXAFS in RMC++ for amorphous materials: Features and advantages

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Reverse Monte Carlo (RMC) modelling combined with diffraction data is a well-established approach for determining the structure of amorphous materials. Although extended X-ray absorption fine structure (EXAFS) data have been incorporated into RMC simulations for more than three decades, their routine use remains limited. This contribution provides a practical overview of how EXAFS constraints can be effectively integrated into diffraction-based RMC modelling using the RMC++ code, with a focus on amorphous systems.

We briefly summarize the connection between EXAFS signals and the pair distribution function and discuss their consistent inclusion in RMC refinements. Particular attention is given to recent developments in RMC++, including the treatment of the energy shift (ΔE_0) and related correction schemes, which improve the stability and reliability of EXAFS-supported fits. A concise overview of other RMC-based approaches capable of handling EXAFS data is also presented to place the method in context.

In this framework, diffraction data provide the primary structural constraints over intermediate and longer length scales, while EXAFS contributes complementary, element-specific information on the local atomic environment. In principle, the simultaneous fitting of multiple datasets reduces model bias and leads to more reliable structural models. The approach is illustrated through examples on amorphous systems, including chalcogenide and metallic glasses. Finally, possible extensions toward the use of molecular dynamics-derived correlation functions and potential-based methods (e.g., RMC_POT) are briefly outlined.

Resonant Total Scattering and Differential PDFs in Reverse Monte Carlo Modeling

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Reverse Monte Carlo (RMC) simulations are widely used to construct atomistic models of materials exhibiting local lattice distortions, chemical disorder, and correlated deviations from average crystallographic structures. By refining large supercell models directly against experimental total scattering data, RMC methods provide structural information that is inaccessible through conventional crystallographic refinement. However, the high flexibility of RMC models also presents a significant challenge: many structurally distinct configurations can reproduce the same experimental data with comparable accuracy, raising important questions about the uniqueness and physical relevance of the refined models.

This talk will present recent advances in improving the reliability and resolving power of RMC refinements through the combined use of total scattering, resonant scattering, and differential pair distribution function (dPDF) analysis. Resonant x-ray scattering enhances chemical sensitivity by tuning the scattering contrast near elemental K and L absorption edges, allowing selective probing of specific atomic pair correlations in chemically complex materials.

Simultaneous refinement against total and dPDFs introduces strong additional constraints on atomistic models, significantly reducing structural degeneracy and improving the uniqueness and interpretability of RMC solutions. The approach enables chemically resolved characterization of disorder, correlated atomic displacements, and nanoscale heterogeneity in complex functional materials.

Applications will be discussed for nanosized catalysts [1–3], multiferroic materials [4,5], and charge-density-wave systems [6–8], demonstrating how resonant total scattering and dPDF analysis substantially extend the capabilities of RMC modeling for studying local structure in disordered materials.

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Characterization of Short Range Order in Ni_4Mo and its disorder-order transition through total scattering and Reverse Monte Carlo modelling.

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Nickel-based superalloys are vital materials in the aerospace industry due to their high strength at high operating temperature[1]. These superalloys are known to obtain their beneficial properties from a dual-phase microstructure[1], consisting of ordered precipitates within a random matrix. Beyond this dual phase nature, Short Range Order (SRO) within the nominally random γ-phase has been observed using Transmission Electron Microscopy (TEM) that could provide further strengthening[2], [3]. However, total scattering has not yet been applied to understand the bulk local structure.

In this study we use Reverse Monte-Carlo (RMC) modelling of neutron PDF data to understand SRO of the simplified model γ-phase Ni_4Mo. Samples prepared under a range of annealing conditions were analysed to explore how SRO evolves across an order-disorder transition observed at this composition. The atomic configurations from RMC modelling were analysed to extract local SRO motifs and quantify them as a function of annealing time. The populations of local environments are compared against random and idealised ordered atomic configurations to explore how the local structure evolves. The SRO evolution shows an increase in motifs associated with the LRO microdomains observed via TEM, supporting a hypothesis that SRO domains act as precipitation points for the long-range order transition[4]. Understanding the nature of this transition provides insight into the nature of local order within these nominally random phases that may improve the properties of these industrially important materials.

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RMC reveals hidden complexity in D_2O Ice VII

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Ice VII is thought to play a role in the water-rich interiors of Jupiter's moon Europa, Saturn's moon Enceladus and other planetary bodies. Although its average cubic structure appears simple, the local structure reveals hidden complexity: individual positions of water molecules forming a complex network via hydrogen bonds. Through coupling Pair Distribution Function and Reverse Monte Carlo modelling by using RMCProfile7, high pressure neutron scattering data allowed to have quantified the atomic and molecular structures of disordered ice VII. The decomposition of the average structure of ice VII into the individual positions of, differently oriented within the crystal lattice, water molecules reveals that the D_2O molecules are displaced along the direction of the polarization vector of each molecule. Incorporating this displacement yields a structural model that more accurately reproduces the D–O distances and D–O–D angles determined for other ordered ice structures. Our results are also supported by DFT calculations confirming that deviations of water molecules from their average crystallographic positions energetically stabilize the structure of ice VII. Our results open new perspectives for structural studies of different forms of ice, their phase transitions treating them as vast clusters of molecules with an average periodic structure but symmetry-free local arrangements [1].

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Inverting PDFs to measure effective interactions decodes complexity in amorphous calcium carbonate

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Understanding the interactions between atoms in materials is crucial to explaining their structure and properties, and is essential for designing new functional materials. Total scattering provides insights into real-space structure via the pair distribution function (PDF), and advances in refinement techniques now yield realistic atomistic configurations even for disordered materials. Yet inverting this structural data to measure underlying interactions remains challenging. Here, we solve this *inverse problem* by matching the PDF obtained using test-particle insertion with that from the traditional distance-histogram approach [1]. Our method is applicable in any material where representative configurations are available, and is especially useful in obtaining coarse-grained effective interactions for mapping complex systems onto well-studied simple models.

In particular, we use this approach to measure effective Ca···Ca interactions in amorphous calcium carbonate (ACC), an important precursor for biomineralization in marine organisms [2]. High-quality configurations consistent with X-ray total scattering data and stable with respect to state-of-the-art interatomic potentials were used as a basis for the inversion. The effective Ca···Ca pair potential has two minima, corresponding to Ca^{2+} ions bridged by one or two oxygens of the carbonate anion. Remarkably, the potential can be mapped to the multi-well Lennard-Jones-Gauss potential studied in computational soft matter, with model parameters that are known to promote structural complexity. This shows that the complex structure of ACC and its metastability as an amorphous phase, both critical to its biological role, are encoded in the geometrically frustrated effective interactions between Ca^{2+} ions.

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RMC Study of Local structure and disorder in Inorganic Halide Lead Perovskite Quantum Dots

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Inorganic lead halide perovskite quantum dots ($CsPbX_3$, X = Cl, Br, I)have emerged as promising materials for light-emitting devices, photodetectors, and photovoltaic applications owing to their outstanding optical properties and defect tolerance. Local atomic structure and disorder critically influence the optoelectronic performance of inorganic halide lead perovskite quantum dots (QDs), yet conventional diffraction techniques provide only average structural information.

In this work, high-energy synchrotron X-ray total scattering, pair distribution function (PDF) analysis, and Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy are combined with Reverse Monte Carlo (RMC) modelling to investigate the local structure of inorganic halide lead perovskite quantum dots. The RMC approach is employed to construct atomistic structural models consistent with the experimental scattering data, enabling the analysis of local atomic correlations beyond the average crystallographic structure. The presentation will focus on local bond-length distributions, PbX6 octahedral distortions, and the influence of halide composition on the local atomic structure. By integrating total scattering, EXAFS spectroscopy, and RMC modelling, this work aims to provide a more comprehensive understanding of local structural disorder in perovskite quantum dots.

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Flexible Polarizable Water Model Parameterized via Gaussian Process Regression

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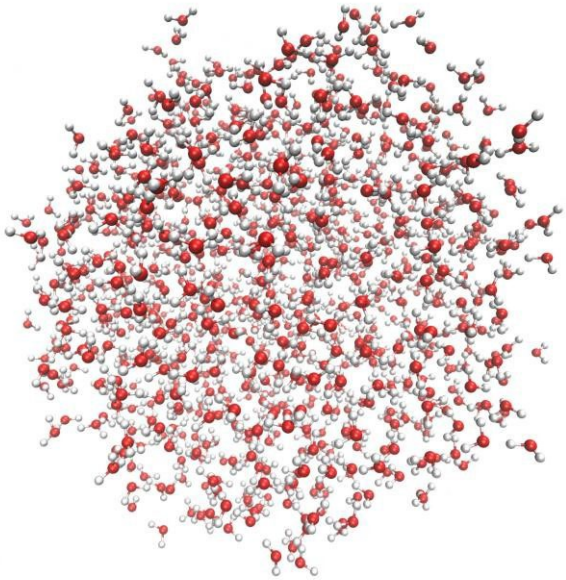
Water is often a crucial component of many molecular simulations. To accurately model chemical reactions at or near water interfaces with classical force fields, it is essential to employ a water model that is both polarizable and flexible.

Here, we present SWM4/Fw, our in-house flexible polarizable water model.[1] The model was optimized using Gaussian process regression, a machine learning technique that predicts the model's properties without requiring additional simulations whenever the force field parameters change. SWM4/Fw reproduces many reference water properties and provides the flexibility needed to model chemical reactions involving bond stretching or breaking, as well as to calculate vibrational spectra. The model is also computationally efficient, owing to the use of an extended Lagrangian with Drude oscillators to represent explicit electronic polarization. Our approach, based on Gaussian process regression, should also be useful for developing other force fields.



Droplet of 1000 SMW4/Fw water molecules

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38 Years of Reverse Monte Carlo Modelling

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Many of the materials that enable modern technologies owe their properties not only to their average crystal structures, but also to the local deviations, disorder and correlations hidden within them. Over the past four decades, total scattering has become an essential technique for revealing this local structure, combining Bragg and diffuse scattering to provide information on both long-range order and short-range atomic arrangements. To extract the maximum insight from such data, we need structural models that are consistent with experiment while still retaining chemical and physical meaning.

Reverse Monte Carlo modelling was introduced by McGreevy and Pusztai in 1988 as a remarkably direct way to build such models. A large configuration of atoms, with the correct composition and density, is adjusted through random moves until the calculated scattering agrees with the experimental data. In the 38 years since its introduction, RMC has developed from a provocative method for modelling disordered systems into a broad family of approaches used to study liquids, glasses, crystalline disorder, magnetic materials, diffuse scattering and increasingly complex functional materials.

In this presentation, I will give a personal view of the first 38 years of RMC: what the original idea made possible, how the community has extended and challenged the method, and what we have learned about both its power and its limitations. I will discuss the importance of combining multiple data sets and constraints, the continuing need to balance experimental agreement with structural realism, and the development of tools such as RMCProfile to maximize the information obtained from total scattering data. Finally, I will look ahead to how RMC-based methods may continue to evolve as experiments, computation and our understanding of disorder become ever more sophisticated.

Molecular RMC on Tetrel-Chalcogenid Clusters with Extreme Nonlinear Optical Properties

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Light-emitting diodes (LED) are highly energy efficient light sources. Light emission takes place in all directions in mainly the visible spectrum without heat loss in the infrared. [1]

Ten years ago, alternative light sources with highly directional irradiation properties have been found. These organotetrel chalcogenide clusters show extreme nonlinear optical properties by irradiation from a continuous-wave laser diode. If the compound consists of an amorphous matrix, a broad band emission in the visible region is seen. This effect is known as white-light generation (WLG). If the sample is crystalline, second-harmonic generation (SHG) takes place. [2,3]

More specific, clusters with a general formula of $((RX)_4Y_6)$ show these characteristics, where R is an organic substituent, X is a group 14 element (Si or Sn) and Y is a group 16 element (S or Se). Depending on the composition the resulting nonlinear optical effect is either SHG, e.g. $((NpSn)_4S_6)$ or WLG such as in $((PhSn)_4Se_6)$. [3-6]

We performed molecular Reverse Monte Carlo modelling of the $((RSn)_4Se_6)$ clusters by fitting X-ray diffraction, extended X-ray Absorption Fine Structure (EXAFS) data and Neutron Diffraction simultaneously. Large distortions are found to be present in the intramolecular structure of Ph- and Cp-decorated clusters. This is suspected to suppress crystallisation. [7]

Results of the molecular Reverse Monte Carlo modelling as well as the inter- and intramolecular arrangements of the clusters will be presented.

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Combining Reverse Monte Carlo Analysis of X-ray Scattering and Extended X-ray absorption Spectroscopy

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Extended X-ray absorption fine structure (EXAFS) spectra contain information about the local, molecular type structure, whereas (X-ray) diffraction (XRD) data reveal the periodic structure or long-range order (crystal structure) of materials. Variations in local and periodic structure greatly influence materials properties and related applications. However, data analysis often is performed independently for EXAFS spectra and diffraction data even if measured simultaneously.

RMC simulations enable the analysis of X-ray scattering (XS) data as well as EXAFS spectra data via partial pair distribution (pPDF) functions obtained from a physical, structural model. In case of nanoparticles and scattering data this approach suffers from the termination of the pPDF's due to the finite size of the particles. This produces artifacts in the computed scattering intensity due to the long-range probing distance of scattering which are eliminated using the Debye scattering equation (DSE) [1, 2]. Simultaneous refinement of XS data and EXAFS spectra of small nanoparticles are thus enabled using a mutual structural model. This method allows the self-consistent extraction of complementary information on local structure contained in EXAFS and long-range order in XS data. However, refinement of raw diffraction data for crystals of larger domain size (larger than about 10 nm or 50.000 atoms) are difficult. A Rietveld code embedded into the RMC code and feedback of the essential structural information between both refinement paths enables the coupled refinement of diffraction and EXAFS data are in this case [3].

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3D Probing of Hidden Nanoscale States in Functional Materials

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Local structure in advanced materials plays an important role in unveiling exotic functionalities and properties. The conventional one-dimensional pair distribution function (1D-PDF) method has been widely applied to investigate local structural distortions beyond the average crystallographic structure. However, a major challenge in 1D-PDF analysis arises from the isotropic powder averaging, which loses the directional information of atomic pairs. Here, we develop a three-dimensional PDF (3D-PDF) method to address this issue. In this approach, total scattering signals are collected from a single-crystal sample, and the experimental data can be reconstructed in full 3D space. As a result, interatomic distance-vector information is retained and can be further analyzed quantitatively using our newly developed 3D-PDF software. By combining the supercell model analysis using RMCProfile, both local and average structural behaviours can be captured quantitatively. This method has been successfully applied to complex functional materials, including those exhibiting ultralow thermal conductivity and superionic behaviours.[1-3] The 3D-PDF total scattering experiment enables straightforward retrieval of diffuse scattering with directional information and can be widely applied to reveal local atomic structural features in various materials.

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RMC-XANES Builder, a flexible workflow for XANES calculations

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RMC-XANES builder is a scientific software to connect atomistic structural models obtained from Reverse Monte Carlo (RMC) simulations with first-principles X-ray Absorption Near-Edge Structure (XANES) calculations. This workflow directly processes RMC-derived structural models to convert them to input files for XANES simulations. The software allows to import large atomic configurations generated by RMC calculations, enable chemically and topologically selective filtering of absorber environments (based on coordination number and neighbor-type combination). The software contains integrated simulation (single and batch mode) tool for theoretical XANES calculation based on FEFF (or optionally FDMNES). Statistical refinement and comparison with experimental data is available as well. The software is open source, written in Python and has a user-friendly GUI to facilitate the usage.

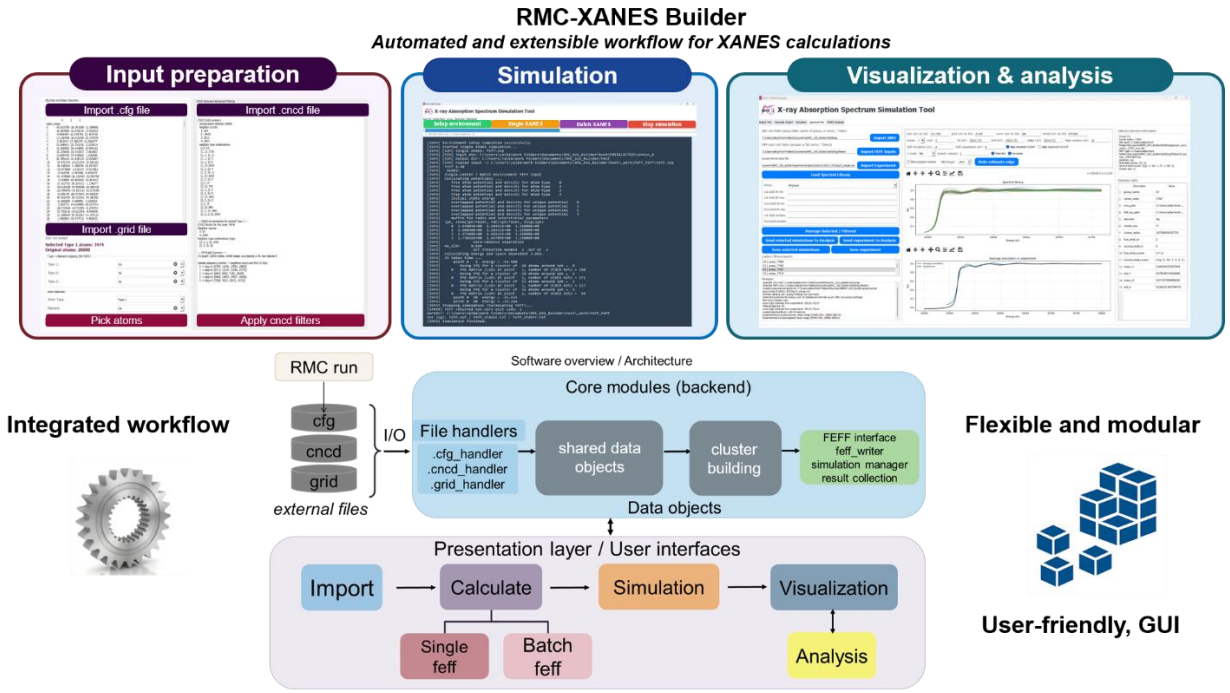

Figure 1 Overview of the X-ray Absorption Spectrum Simulation Tool, showing its modular software architecture and main user-facing workflows.

Combining Exhaustive Symmetry and Attention Based Learning for Phase Transition Studies

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Abstract

Determining the atomic structure of materials along the phase transition pathway using either neutron or x-ray powder diffraction is typically a labor-intensive process of iterative structural design and refinement that requires expert domain knowledge. Such bottom-up approaches either do not fully leverage the existing knowledge within the problem domain or are overly tailored to specific systems thus compromising the generalizability and present a major bottleneck for high throughput analysis. Here we present a top-down deep learning approach for structure determination by combining group-theoretical methods for an exhaustive list of symmetry candidates and a multi-head attention convolutional neural network for classification. The developed workflow, termed XsymNet, is demonstrated to reliably identify the structure (including space group, lattice, and atomic positions) along the displacive phase transition pathway for several representative systems with both simple and complex phase diagrams. Both high-resolution neutron and X-ray powder diffraction data have shown to work robustly with XsymNet for structure identification. Our work highlights the power of combining physics domain knowledge with the non-linearity of neural networks to solve complex phase diagrams, and further, this framework is readily extendable for use with single crystal and diffuse scattering experiments.

Abstracts of Posters

(in alphabetical order)

Smart Solar Breakthrough: Machine Learning Powers Next-Gen $CsSnI_3$/Si Tandem Cells

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Abstract

Tandem solar cells enhance the absorption of photons by utilizing materials that have different band gaps, allowing them to exceed the efficiency limits set by standard single-junction cells. In these configurations, the upper cell captures high-energy photons, whereas lower-energy photons are transmitted to the lower cell for additional conversion. This research presents a computational study of a two-terminal tandem solar cell that merges a lead-free $CsSnI_3$ top cell with a silicon bottom cell. The examination was carried out using SCAPS-1D simulations, which were improved with machine learning techniques to fine-tune device parameters like layer thickness and doping levels to achieve current matching and minimize losses from recombination. The $CsSnI_3$ absorber was meticulously adjusted to improve charge carrier behavior and optimize optical absorption, while the silicon subcell was modeled based on the filtered light spectrum from the top cell. The optimized tandem configuration reached a PCE of 29.68%, featuring a Voc of 1.675 V, a Jsc of 20. 47 mA/cm², and a FF of 86.53%. These findings suggest the potential of machine learning-enhanced design in the development of high-efficiency, lead-free perovskite/silicon tandem solar cells. This methodology not only achieves impressive efficiency but also promotes sustainable and cost-effective photovoltaic technologies for future solar energy advancements.

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Optimizing lead-free $FASnI_3$-based perovskite solar cells using SCAPS-1D: A numerical Study with different Hole Transport Layers (HTLs)

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Abstract

In this study, a lead-free perovskite solar cell with the architecture FTO/TiO_2/$FASnI_3$/PTAA/Au was numerically simulated using the SCAPS-1D software. The $FASnI_3$ absorber layer was initially calibrated based on available experimental data, resulting in a power conversion efficiency (PCE) of 7.14%, closely aligning with the experimental J–V characteristics. To enhance device performance, key parameters such as absorber thickness, defect density, and carrier concentration were systematically optimized. Furthermore, the impact of various hole transport layer (HTL) materials including SnS, $MoTe_2$, MoOx, Spiro-OMeTAD, and CuSCN was investigated to identify efficient alternatives to the commonly used PTAA. The simulations revealed that improvements in both structural and interfacial properties significantly enhance device performance. Notably, the configuration employing MoOx as the HTL achieved a remarkable PCE exceeding 36%, demonstrating its potential for high-efficiency and environmentally friendly photovoltaic applications. This study offers valuable insights into the design and optimization of lead-free perovskite solar cells and emphasizes the critical role of interface engineering in the development of next-generation solar technologies.

Keywords : $FASnI_3$, SCAPS-1D, lead-free perovskite, numerical simulation, HTL optimization.

Experimental and DFT study of Ce-doped $LaNiO_3$ perovskite for photo-assisted oxidation processes

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Abstract. This study investigates the structural, electronic, and optical properties of Ce-doped $LaNiO_3$ perovskite nanomaterials ($La_{1-x}Ce_xNiO_3$, where x = 0.00, 0.03, 0.05) synthesized via a co-precipitation method. X-ray diffraction (XRD) analysis confirms that the materials maintain a dominant rhombohedral structure, with only trace amounts of CeO_2 and NiO secondary phases detected. UV-Vis spectroscopy reveals a red shift in the optical absorption edge as Ce content increases, with optical transition energies decreasing from 1.70 eV (x = 0.00) to 1.61 eV (x = 0.05). These experimental findings are supported by Density Functional Theory (DFT) calculations, which indicate that while the metallic character of $LaNiO_3$ is preserved, Ce incorporation perturbs Ni-O hybridization and reshapes local electronic states.
Photoluminescence (PL) analysis demonstrates a significant decrease in emission intensity with increasing Ce concentration, suggesting suppressed charge-carrier recombination and improved charge separation. Furthermore, energy-level alignment estimates show that the hole energy levels (E_{h+}) for all samples are positioned more positively than the water oxidation potential (+1.23 V vs NHE), indicating a strong oxidative potential favorable for visible-light-driven processes. Among the studied compositions, the 3% Ce-doped sample exhibits the most balanced performance in terms of optical transition energy, carrier transport, and energy-level alignment. These results position Ce-doped $LaNiO_3$ as a promising candidate for photo-assisted oxidation applications, such as solar-driven water splitting and pollutant degradation.

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Probing the local lithium environment in Li-rich and Mn-rich disordered rocksalt materials for battery applications: a combined neutron and X-ray Pair Distribution Function study

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Keywords Disorder, PDF, Oxyde, Oxyfluoride, Modelling

Abstract

Lithium-rich compounds of the general formula $Li_{1+x}(M,M')_{1-x}(O,F)_2$ (where M and M' are transition metals, x> 0) exhibiting a disordered rock-salt structure have been of great interest to the battery community for about a decade. A representation of this type of structure is shown in Figure 1. When used as positive electrode materials in lithium-ion batteries, these compounds achieve stable specific capacities approaching 175 mAh/g while being free of critical elements such as cobalt and nickel, making them very attractive for use in electric vehicles. [1] These compounds are generally metastable, especially when containing significant amounts of fluorine, and are obtained by synthesis methods that “freeze” the cationic and anionic disorder (high temperature synthesis followed by quenching, mechanosynthesis, microwave heating synthesis, etc.).

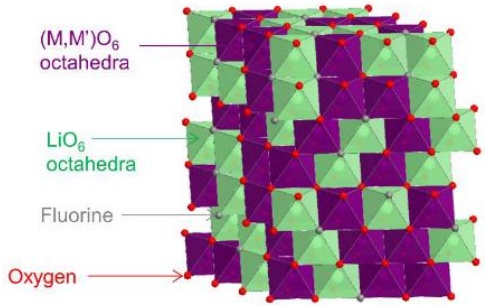

Figure 1. Three-dimensional representation of a disordered rocksalt structure

Therefore, a simple average rock-salt structure frequently does not capture the true local (dis)order, which is often considerably more complicated. Accurate descriptions of both local and average long-range structure in these materials are critical for any detailed understanding of the transport mechanisms and electrochemical performance.

In this context, the $Li_{1.25}Mn_{0.5+y/2}Nb_{0.25-y/2}O_{2-y}F_y$ (LMNOF) system with a rock-salt type structure is studied, and particularly two compounds: the parent oxide $Li_{1.25}Mn_{0.5}Nb_{0.25}O_2$, and the oxyfluoride $Li_{1.25}Mn_{0.7}Nb_{0.05}O_{1.6}F_{0.4}$. These two compounds were selected to investigate the impact of fluorine on the local structure of these materials and, consequently, on the pathways of lithium deintercalation and reintercalation. PDF is a valuable tool to investigate the local structure because it gives access to distances between ion pairs in the structure. Neutron PDF data is valuable to get information on Li while X rays PDF data gives us information on Mn and Nb in the structure. Combining both in a joint analysis using big box modelling with RMCProfile [2] provides a full picture of the local structure in the LMNOF materials.

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RMC-EXAFS Study of Local Structure in WO_3 Nanoparticles

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Tungsten(VI) oxide (WO_3) is extensively investigated for solar energy applications due to its pronounced photochromic behavior [1]. The reversible color changes in WO_3 are associated with modifications in its electronic structure and local atomic arrangement [1]. Consequently, X-ray absorption spectroscopy provides an effective approach for probing these transformations.

WO_3 nanoparticles (NPs) were synthesized via the polyol process [2]. The synthesis route was modified by the addition of an oxidizing reagent. X-ray diffraction measurements yielded an average crystallite size of 3–5 nm. Protonation was induced through hydrogen spillover on metallic indium in an acidic environment, resulting in protonated $HxWO_3$ NPs.

X-ray absorption spectroscopy at the W L_3-edge was conducted at 300 K at the DESY PETRA III P64 and P65 beamlines (Hamburg, Germany) [3,4]. EXAFS spectra were recorded for a series of WO_3 nanoparticle samples and a microcrystalline reference in both protonated and non-protonated states. Structural analysis was performed using the reverse Monte Carlo (RMC) approach augmented by an evolutionary algorithm [5].

RMC modeling of the EXAFS spectra provided insight into the evolution of distortion in the W–O first coordination shell across different samples. The results show that protonation causes the tungsten atoms to shift toward the center of the octahedra, resulting in a reduction in the distortion of the WO_6 octahedra.

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A Mixed Ligand Approach to Amorphisation Control in **Z**eolitic **I**midazolate **F**rameworks (ZIFs)

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Amorphous and glassy metal–organic frameworks (MOFs) represent an emerging class of materials with tunable local structure and unique functional properties, yet the structural origins of framework amorphisation remain poorly understood. [1] My project explores a mixed-ligand strategy for controlling amorphisation behaviour in zeolitic imidazolate frameworks (ZIFs), using systematic linker substitution to probe how local disorder influences framework stability and collapse pathways using ZIFs with large ring structures.

The work will combine synthesis, total scattering, and pair distribution function (PDF) analysis to investigate structural evolution beyond the limits of conventional crystallography. By developing a foundational understanding of how mixed-linker environments affect short- and medium-range order, my project aims to establish a platform for future reverse Monte Carlo (RMC) modelling and computational analysis of the resultant amorphous MOF structures.

This poster introduces the early-stage methodology, experimental design, and long-term vision for integrating advanced PDF data processing and atomistic modelling into the study of amorphous ZIFs.

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RMCProfile7: Investigation of the local structure of hydrogenated High Entropy Alloys

Joanna Grelska

Multielement High Entropy Alloys has emerged as promising candidates for solid-state hydrogen storage. Those materials crystalize in two main cubic structures: fcc or bcc, with hydrogen atoms in tetrahedral or octahedral sites. However, its structural complexity cannot be well understood only by looking at the average structure, especially when its hydrogenated forms are investigated. Some of the high entropy alloys properties, for example hydrogen capacity or chemical stability can be linked to the specific local structure. Therefore, more advanced analysis that goes beyond regular crystallographic approach is required.

One of the possible approaches to probe local structure is by pair distributions functions, obtained from experimental X-ray or neutron high quality data, or calculated in theoretical model. In the study, Reverse Monte Carlo method implemented in RMCProfile7 software is used to probe the local structure of High Entropy Alloys. RMCProfile7 employs big box modeling where atoms in initial average positions are refined by accepting or rejecting small moves. The simulation process continues until model calculated structure factor, pair distribution function and Bragg intensity data give the best fit to the experimental data. Such models are later analyzed in terms of local atom correlations, average coordination number or specific elements short range order.

The study of High Entropy Alloy (TiVNb)85Al5Mo10 is presented and its local structure compared to bulk TiVNb. Despite the multielement composition, the first alloy is characterized with smaller unit cell parameters and more effective reversable hydrogen capacity[1]. Another hydrogenated High Entropy Alloys Al10(TiVZrNbHf)90 and TiVZrNbHf emphasizes the addition of Al on local structure and hydrogen storage. Combing the X-ray and neutron diffraction data enables the determination of deuterium positions as well distances of metals with similar atomic numbers. Modeling in RMCProfile7 allows to obtain a wealth of information from ordinary experimental data.

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Comparative study of ZrV_2O_7 and ZrP_2O_7 by lattice dynamics simulations and neutron total scattering measurements: exploring the different thermal expansivities

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[3] ISIS Neutron and Muon Facility, Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxfordshire, OX11 0QX, UK
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ZrV_2O_7 is a cubic crystal that exhibits negative thermal expansion (NTE). Its crystal structure consists of interconnected ZrO_6 octahedra and VO_4 tetrahedra. However, ZrP_2O_7, which possesses an identical crystal structure, shows only positive thermal expansion (PTE). Here, we report work in progress aimed at identifying the common dynamical features underlying their contrasting thermal expansion behaviors. We analyze the flexibility of this structure using calculations of lattice dynamics by density functional theory, paying particular attention to the flexibility both within the polyhedra and between neighboring polyhedra. It is found that transverse acoustic modes and low-frequency optic modes, which are associated with the *tension effect* [1], make the largest contributions to NTE. Although these modes are present in both materials, significant differences in the overall Grüneisen parameters are found between ZrV_2O_7 and ZrP_2O_7. We are performing reverse Monte Carlo (RMC) modeling of neutron total scattering data to quantitatively analyze the vibrational patterns of P–O–P linkages in ZrP_2O_7. These findings may provide a useful reference for understanding how substitution by different elements with the same valence state can be used to tune NTE behavior.

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Total Scattering and RMC Insights into Disorder in the Bismuthinite-Aikinite Series

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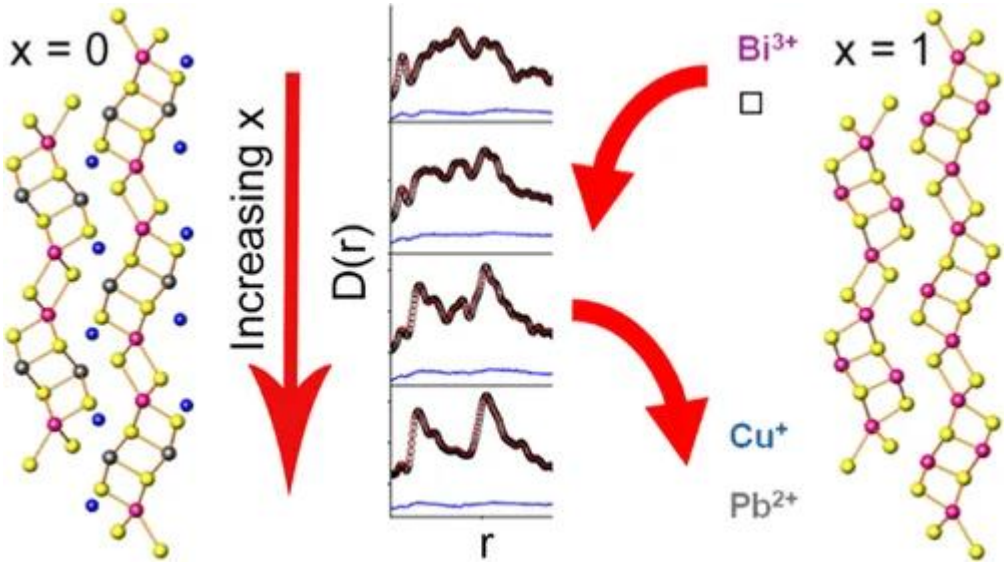
This study employs "big box" Reverse Monte Carlo (RMC) modeling to resolve the local structural origins of ultralow thermal conductivity in the bismuthinite–aikinite series ($Cu_{1-x}\square_xPb_{1-x}Bi_{1+x}S_3$). While traditional crystallographic averages mask the complexity of these phases, our large-scale RMC configurations—fitted to total scattering data—capture the nuanced interplay between Cu-vacancy (□) ordering and Pb/Bi cation distribution. Our results reveal that the material's glass-like thermal transport arises from significant local-scale structural frustration and anharmonicity. By utilising RMC to visualise real-space distortions across thousands of atoms, we demonstrate that these collective disorders act as potent phonon scatterers. This work underscores the necessity of "big box" modeling for identifying the structure-property relationships in complex minerals where local deviations from the mean dictate macroscopic performance.



Title

Crystal PDF Full-space Refinement: An RMCPOW-derived approach for high-precision structure analysis of crystalline materials

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Pair distribution function (PDF) analysis has become a powerful tool for investigating local atomic structures not only in disordered but also in crystalline materials. Particularly for crystalline materials, attempts have been made to describe deviations from the average structure (local distortions) by utilizing the high real-space resolution of the PDF. However, in conventional crystal structure analysis based on the PDF, the computational cost increases rapidly as the fitting range is expanded to longer real-space ranges, making simultaneous analysis of both local and average structures difficult.

We present Crystal PDF Full-space Refinement, a high-precision structure refinement framework derived from the scattering intensity formalism implemented in RMCPOW. In contrast to conventional small-box PDF refinement approaches, Crystal PDF Full-space Refinement directly calculates total scattering intensities from explicit atomic configurations in reciprocal space and performs refinement in full real space through the Fourier transform. The method enables simultaneous treatment of Bragg and diffuse scattering contributions while preserving crystallographic constraints. By utilizing direct atomistic modeling and reciprocal-space-based PDF calculations, Crystal PDF Full-space Refinement achieves highly sensitive refinement of subtle structural variations.

In this presentation, we will introduce the methodology and refinement algorithm of Crystal PDF Full-space Refinement, including its relationship to the RMCPOW formalism. We will also present structural analyses of two representative materials performed using Crystal PDF Full-space Refinement. The first example concerns Li-rich layered oxide (LLO) cathode materials for lithium-ion batteries, in which site occupancies vary during charge–discharge processes. Crystal PDF Full-space Refinement enabled highly precise determination of site occupancies and successfully revealed characteristic structural behavior while preserving the layered crystalline framework during electrochemical reactions.

The second example concerns Si-Ge powder samples transformed into crystalline–amorphous mixtures through prolonged ball milling. In this sample, the Bragg peak intensities from the crystalline phase are extremely weak due to the dominant amorphous phase. Crystal PDF Full-space Refinement successfully refined the structure of the trace crystalline phase. Furthermore, it enabled the extraction of the PDF contribution from the amorphous component.

These results demonstrate that Crystal PDF Full-space Refinement provides a versatile framework for high-precision structural analysis of complex crystalline materials containing disorder, multiphase coexistence, and local structural heterogeneity.

Spin dynamics in the trimer-host compound $Dy_3Ru_4Al_{12}$

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Anorganic quantum materials with kagome lattice structure harbor manifold quantum phenomena, ranging from flat band electronic structures to dynamically disordered states, such as spin liquids. Also, long-range ordered phases of matter on the Kagome lattice have peculiar properties due to the presence of various magnetic ground states that are nearly degenerate in energy.

In $Dy_3Ru_4Al_{12}$ (space group $P6_3/mmc$), the Dy^{3+} ions form breathing kagomé layers that are composed of two different sizes of corner-sharing triangles [1,2]. Below T_N = 6.5 K, $Dy_3Ru_4Al_{12}$ enters an antiferromagetically ordered phase with propagation vector $\boldsymbol{q}$ = (1/2, 0, 1/2) [1]. Polarized neutron diffuse scattering experiments were performed on the DNS diffractometer at the Mayer Leibniz Zentrum in Garching, Germany. Crystals were polished to thin slices of dimensions of 3.0×0.8×0.15 mm^3 to reduce neutron absorption caused by the Dy element [4].

An exotic diffuse scattering pattern in the L = 0 plane was observed at T = 8.5 K. We report here that the scattering pattern can be described by a minimal model that includes five exchange parameters, consistent with long-period magnetic interactions due to the Ruderman Kittel Kasuya Yosida (RKKY) interaction in this material family.

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Anomalous x-ray scattering to strengthen partial local atomic investigations in reverse Monte Carlo analyses

S. Hosokawa

To investigate local atomic structures on multi-component non-crystalline materials, reverse Monte Carlo (RMC) modeling is widely used. Although the validity of the modeling can be obtained by the increase of the number of experiments for the target material as well as the improvements of the experimental quality, only a few efforts were performed so far. For those, we have worked on anomalous x-ray scattering (AXS) technique at the large synchrotron radiation facility of the ESRF for about 20 years [1]. Recently, a more sophisticated setups were installed at a more intense undulator device in the SPring-8 [2], and we expected to obtain more reliable experimental data for the RMC analysis. In this presentation, we introduce the recent improvements at the SPring-8 such as the remarkably improved energy resolution for the scattered x-rays using a LiF crystal and experimentally obtained anomalous terms of atomic form factors. These efforts made the output of differential data close to the absorption edges much reliable and gave the partial results of the RMC analysis quantitatively excellent. As an example, we will show the RMC results on a Zr50Cu50 metallic glass.

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Design of Two-Phase Hyperuniform Photonic Materials for Complete Band Gaps

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Aperiodic photonic materials are promising candidates for robust and isotropic light control. However, the structural conditions required to obtain a complete photonic band gap (CPBG), where light cannot propagate in any direction or polarization, remain unclear. Hyperuniformity describes suppressed large-scale density fluctuations and serves as a descriptor for CPBG formation [1]. In stealthy disordered hyperuniform structures, whose structure factor vanishes over a finite range of wave vectors, [2] showed that such systems support large CPBGs, suggesting that hyperuniformity, short-range geometric order and uniform local topology contribute to gap formation. Recent studies show that the final dielectric geometry, not only point positions, strongly affects band gaps. The introduction of additional air cavities induces CPBGs in quasiperiodic approximants lacking one [3], while elliptical dielectric rods enhance TM gaps in stealthy hyperuniform structures, unlike in periodic lattices [4]. To account for dielectric-air geometry beyond cavity positions alone, we use the two-phase formulation of hyperuniformity, which treats the structure as a heterogeneous two-phase medium rather than a point pattern [5].

Using this framework, our preliminary two-phase analysis evaluates the volume-fraction order metric $\bar{\mathrm{B}}_{\mathrm{V}}$ as a function of the dielectric volume fraction Φ_2 and radius ratio $\eta = \mathrm{w}_2/\mathrm{w}_1$, where w_1 and w_2 denote the radii of the primary and additional air cavities respectively. We identify an optimal regime with significantly reduced B_{V} compared to the equal-radius configuration $\eta = 1$ (Fig. 1(a)), whose corresponding low-$\bar{\mathrm{B}}_{\mathrm{V}}$ structures (Fig. 1(b)) appear to combine dielectric networks favorable to TE gaps and dielectric spots favorable to TM gaps compare to high-$\bar{\mathrm{B}}_{\mathrm{V}}$ structures (Fig. 1(c)). This suggests that two-phase geometry reveals correlations hidden at the point-pattern level and motivates Reverse Monte Carlo design of hyperuniform photonic materials with anisotropic dielectric rods.

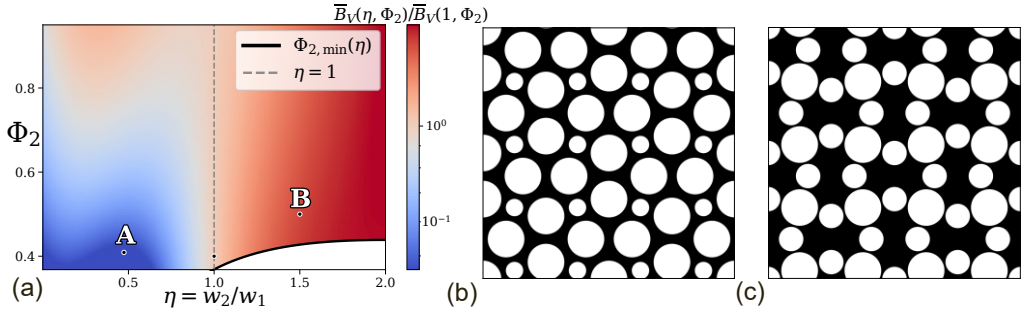

Figure 1: (a) Normalized volume-fraction cumulative-average order metric $\bar{B}_V$ of the Shastry-Sutherland lattice - (b) Structure corresponding to configuration A located in the low-$\bar{B}_V$ region – (c) Structure corresponding to configuration B located in the high-$\bar{B}_V$ region.

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Tracking the Amorphous-to-Crystalline Transition in Solvothermal Sb_2S_3: Evolution of Short- and Long-Range Order

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Controlling the amorphous-to-crystalline transition in Sb_2S_3 is critical for unlocking its potential in next-generation battery anodes [1]. Unlike its crystalline counterpart, amorphous Sb_2S_3 offers superior ion diffusion kinetics and volume-buffering capacity [2]. Yet, the precise local atomic arrangement of these non-periodic phases remains unresolved due to the inherent limitations of conventional long-range crystallography.
Sb_2S_3 powders were synthesized via solvothermal route. By varying several syntheses parameters, we isolated the complete amorphous-to-crystalline phase transition. As illustrated in Figure 1, this evolution is accompanied by a dramatic morphological transformation ranging from amorphous nanospheres stabilized by precursor residue through elongated irregular nanoparticles to highly crystalline bundles of nanowires). Synchrotron X-ray Powder Diffraction (MSPD) and Rietveld refinement robustly quantify only the long-range order of the crystalline Sb_2S_3. Conversely, Raman spectroscopy captures the progressive ordering of the local Sb-S coordination.
While our multimodal dataset details the morphological and long-range structural

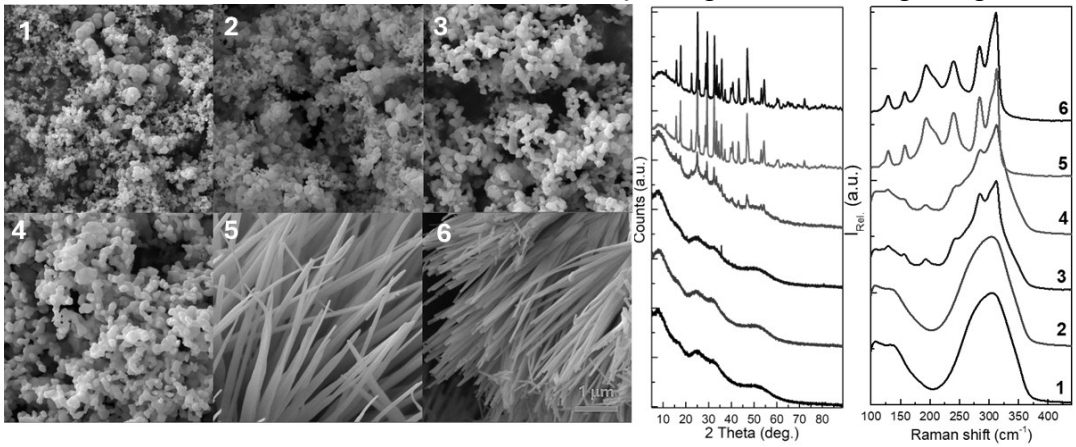

Figure 1: SEM scans, XRD and Raman spectra of solvothermal synthesized Sb_2S_3 powders.

evolution, the definitive 3D atomic configuration of the amorphous Sb_2S_3 precursors remains obscured. This rich experimental foundation is primed for advanced computational techniques. We aim to explore Reverse Monte Carlo (RMC) modeling to bridge our diffraction and spectroscopic data, completely reconstruct the short-range disorder, and definitively establish the vital structure-property relationships.

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Investigation of the local electronic structure and chemical bonding in Pd- and Pt-based bulk metallic glasses by X-ray spectroscopy.

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This study investigates the role of chemical interactions and local electronic structure in the glass-forming ability of bulk metallic glasses (BMGs). Characterizing both the local and extended atomic structure remains a major challenge in the study of metallic glass physics. Short-range ordering and clustering motifs play a crucial role not only in the vitrification process but also in determining the properties BMGs. Pd- and Pt-based BMG systems present an interesting challenge for understanding their thermodynamic behavior, despite their similar kinetic and chemical characteristics. Thermodynamically, Pd–Cu–Ni–P behaves as a much stronger liquid than Pt–Cu–Ni–P, exhibiting a faster decrease in configurational entropy near the glass transition temperature (T_g). However, both systems display similarly fragile kinetic behavior, characterized by a rapid non-linear increase in viscosity in the vicinity of T_g. This apparent contradiction suggests that additional factors, such as short-range order, cluster connectivity, and electronic or chemical structure, must be considered. Previous studies using high-energy X-ray diffraction investigated the atomic structure and revealed changes in cluster types and their connection schemes upon substitution of Pd with Pt [1–2]. These structural variations were correlated with differences in thermodynamic fragility and mechanical brittleness.

The presented experimental study focuses on chemical interactions and modifications of the local electronic structure caused by compositional variation in the systems. X-ray absorption spectroscopy and X-ray photoelectron spectroscopy were employed to obtain element-specific and local information. The density of valence electron states, partial atomic charges, and interatomic charge transfer were analyzed to assess the nature of chemical bonding and to clarify the roles of individual elements in chemical interactions and electronic structure. Generally, chemical interaction in the Pt–(Pd)–Cu–Ni–P system has a notable covalent character, as Pd and Pt have a depleted local electron density, while Cu atoms possess effective negative charge, compared to the reference pure metals. It was found that Pt substitution with Pd results in a gradual buildup of negative effective partial charge on P atoms, which seems to be compensated by depletion of the Ni local electron density. The results are expected to deepen the understanding of the chemistry of BMGs and provide valuable insights for future structural models of metallic glasses.

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Local Structural Analysis of Amorphous Ce–Mn Alloys by X-ray Total Scattering and RMC Simulation

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Amorphous Ce–Mn alloys prepared by a high-rate DC sputtering method have attracted considerable attention as a simple binary system exhibiting a wide variety of physical properties depending on composition[1]-[7]. In the Ce-rich region, these alloys show characteristics of strongly correlated electron systems, whereas in the Mn-rich region they exhibit anomalously large thermal expansion near room temperature. For example, amorphous $Ce_{25}Mn_{75}$ shows a thermal expansion coefficient of approximately 60×10^{-6} K^{-1}[8], which is significantly larger than typical values observed in amorphous alloys. Such diversity in physical properties is considered to originate from differences in the local atomic and electronic structures inherent to amorphous systems; however, the detailed atomic arrangement remains insufficiently understood.

In this study, we investigate the local structure of amorphous Ce–Mn alloys by means of X-ray total scattering measurements combined with reverse Monte Carlo (RMC) simulations.

The structure factor $S(Q)$ is derived from the experimental diffraction data and used as an input for RMC analysis to construct three-dimensional atomic configuration models. Furthermore, the radial distribution function $G(r)$ is evaluated to obtain local structural information such as interatomic distances and coordination numbers.

In this presentation, we will discuss the relationship between the local atomic structure and the composition-dependent physical properties of amorphous Ce–Mn alloys based on these analyses.

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Element-Specific Local Distortions in the High-Entropy Oxide (MgCoNiCuZn)O

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High-entropy oxides are compounds in which five or more elements share a common cation sublattice with equal or near-equal probability [1]. By deliberate selection of the constituent elements, the properties of the compound can be tuned or fundamentally altered. In this study, we investigate the high-entropy oxide (MgCoNiCuZn)O, first reported by Rost et al. [2].

By design, high entropy materials exhibit strong compositional disorder [3]. Combined with variations in size, valence and bonding preferences of the constituent elements, such disorder creates opportunity for local structural distortions. To probe these distortions, EXAFS spectroscopy has proven to be a reliable and robust technique. However, the analysis of EXAFS spectra of multicomponent compounds using conventional approaches are often challenging. The reverse Monte Carlo method, on the other hand, allows simultaneous fitting of multiple absorption edges while considering contributions up to distant coordination shells, which makes this method particularly advantageous for investigating materials that contain multiple elements [4].

X-ray absorption spectra at the Co, Ni, Cu, and Zn K-edges were analyzed using multi-edge reverse Monte Carlo simulations to determine the local atomic structure [4]. In (MgCoNiCuZn)O, metal atoms exhibit octahedral coordination by six oxygen atoms. NiO_6 and ZnO_6 octahedra show only weak distortion, whereas CuO_6 octahedra display clear first-order Jahn-Teller distortion, consistent with the Cu^{2+} oxidation state and previous report [2]. A local distortion around Co atoms is also observed; although previously proposed [2], it is demonstrated experimentally here for the first time.

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Whole-nanoparticle-ensemble refinements of compositionally complex systems from X-ray pair distribution function data *via* the Reverse Monte Carlo method

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Compositionally complex nanomaterials, which consist of five or more elements randomly mixed in a solid solution structure, have emerged as prospect catalysts with tunable properties[1]. However, their multi-element nature complicates comprehensive structural analysis through conventionally applied methods such as powder diffraction and X-ray absorption spectroscopy. Total scattering and pair distribution function (PDF) analysis has proven an excellent tool for structural characterization of compositionally complex and nano-sized materials[2, 3]. Regardless, PDF analysis has not been explored for identification of chemical short-range order (CSRO) and compositional inhomogeneities in nanoparticles, as these structural effects are difficult to describe through commonly employed small-box modelling methods.

We demonstrate a methodology for atomistic whole-nanoparticle-ensemble refinements of compositionally complex nanoparticles through the Reverse Monte Carlo (RMC) method. We analyze a series of nanoparticle systems of increasing compositional complexity (Pt, PdPt, PdPtRh, PdPtRuRh and IrPdPtRuRh) to probe the robustness of the technique. Refinement results of NP ensembles of different compositional ordering, including core@shell, compositional gradient and fully random structures are compared to determine which model best describes the synthesized particles. By introducing atom-type swapping in the refinement algorithm, the presence of compositional ordering and CSRO is investigated. The refinement results indicate concentration gradients and local atomic clustering, a feature which is further investigated through state-of-the-art high-resolution electron microscopy and spectroscopy. This work presents a new approach to the identification of CSRO and compositional inhomogeneities in nanoparticle systems through PDF analysis, enabling identification of structural effects that elude conventional characterization techniques. Furthermore, our results emphasize the challenges associated with comprehensive structural analysis of compositionally complex nanomaterials.

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Barocaloric Materials for Solid-State Cooling

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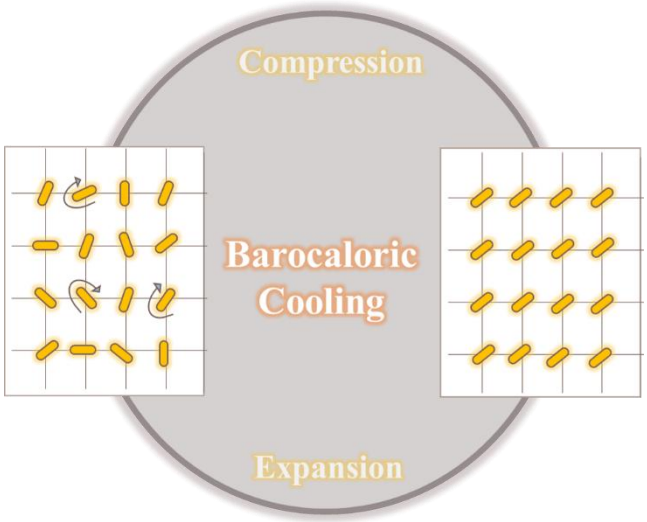
Traditional cooling methods employ conventional vapor compression techniques. However, these systems rely upon materials such as chlorofluorocarbons which are a major source of greenhouse emissions and ozone layer depletion[1]. Thus, there is an urgent need for a more environmentally friendly system. Caloric materials can be regarded as a sustainable alternative to the current refrigeration methods[2]. Among the various caloric materials, barocalorics—materials that exhibit reversible thermal changes in response to an applied hydrostatic pressure[3], is one of the least explored areas. The present study aims at investigating a range of materials particularly plastic crystals for their barocaloric properties. Plastic crystals exhibit reversible order–disorder phase transitions in solid state and this is associated with a large entropy change[4]. The work attempts to understand how the geometry and nature of counter cations or anions contribute to the different barocaloric properties. Following the synthesis of the plastic crystals, their caloric properties will be determined using single crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), and high-pressure differential scanning calorimetry.



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Hidden structural complexity in Ammonia Borane

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Ammonia borane (BH_3NH_3) is a promising hydrogen storage material crystallizing at room temperature in the tetragonal space group I4mm [1, 2]. Despite its relatively simple average structure, the compound exhibits significant orientational disorder related mainly to the hydrogen atoms. This disorder originates from the mismatch between the crystallographic fourfold symmetry and the intrinsic trigonal symmetry of the BH_3 and NH_3 groups [2]. To investigate the local structure, synchrotron total scattering measurements were analyzed using Pair Distribution Function (PDF) methods combined with Reverse Monte Carlo (RMC) simulations performed with the RMCProfile7 program [3]. The resulting big-box configurations reproduce the average structure while revealing local molecular orientations and preferred hydrogen positions without any molecule decomposition [4]. Good agreement with the experimental data was obtained even for short B–H, N–H, and B–N distances, which are difficult to reproduce in PDF analysis.

Single-crystal diffraction at 100 K revealed weak satellite reflections below the phase transition temperature, confirming the presence of a modulated phase. Their low intensity, however, prevented a full refinement. Comparison of the 100 K powder pattern with the literature model shows clear discrepancies, demonstrating that the low temperature phase cannot be described by the average structure alone [1, 2]. To account for these differences, a modulation-based structural model was developed. It introduces orientational shifts of the NH_3 groups and reproduces the main features of the experimental diffraction pattern, showing that the 100 K behavior of BH_3NH_3 results from a combination of NH_3 group disorder and periodic molecular modulation. RMC calculations independently support this picture, revealing pronounced disorder within the NH_3 groups, consistent with the single-crystal results.

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Characterization of the Solvation Shell of Pyranose and Furanose Forms of Hexose Molecules Using Classical and ab initio Molecular Dynamics

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Saccharides serve as fundamental building blocks for essential biomolecules, playing critical roles in biological processes such as molecular recognition, structural stabilization, and the cryoprotection of living cells. [1] Central to these processes are the foundational units themselves – the monosaccharides. Since these phenomena occur naturally in aqueous environments, understanding the behavior of monosaccharides in water is crucial. Although monosaccharides are generally considered hydrophilic compounds, they have substantial hydrophobicity that varies with their structure. To complement this interplay of hydrophilic and hydrophobic regions, the solvation shell of these molecules is determined by a competition between intramolecular hydrogen bonds and intermolecular ones formed with the surrounding water molecules.

In this presentation, biologically relevant hexose isomers – specifically D-glucose, D-mannose, D-galactose, and D-fructose, including both the pyranose and furanose forms of the latter – are considered. Despite their highly similar molecular structures, their fundamental properties, such as water solubility, can differ significantly. We characterize the hydration of these monosaccharide molecules by calculating key properties that reveal their underlying differences. Combining classical and *ab initio* molecular dynamics simulations provides a robust and comprehensive foundation for our findings. [2]

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Intermetallic phases and liquid alloys in Pt-Ga SCALMS by pair distribution function analysis

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Supported Catalytically Active Liquid Metal Solutions (SCALMS) have emerged as a promising class of materials combining the advantages of heterogeneous and molecular catalysis. Nanosized droplets of liquid metal are supported on porous metal oxide supports [1]. Pt–Ga SCALMS on SiO_2 exhibit high activity in the propane dehydrogenation reaction, with hydrogen pretreatment significantly affecting the catalyst performance and stability. However, gradual deactivation is still observed, likely caused by structural changes, the formation of Pt_x–Ga_y phases, disordering processes or phase separation during catalysis [2]. *Ex situ* PDF analyses were performed on as-synthesized and post-catalysis Pt–Ga SCALMS with varying Ga/Pt ratios on data from P02.1, PETRA III. The results reveal that as-synthesized catalysts contain amorphous β-Ga_2O_3, as well as Pt_{fcc} nanoparticles and suspect minor amounts of a liquid metal phase, contributing to the shoulder in the difference PDF (dPDF) of the $Ga_{177}Pt$ SCALMS (red dashed line, Figure 1). The dPDF is yielded by subtraction of the signal of the SiO_2 support from the sample data prior to PDF calculation. Under catalytic reaction conditions, the Pt_{fcc} nanoparticles convert completely into a Pt_2Ga alloy. $Ga_{177}Pt$, with the highest Ga/Pt ratio investigated, shows the least formation of the alloy, aligning with their highest catalytic performance [3]. Further *in situ* PDF experiments are under planning. We hope to achieve deeper insight into the structural dynamics of these liquid metal solutions via RMC modelling to optimize the Pt-Ga SCALMS catalytic activity and stability further.

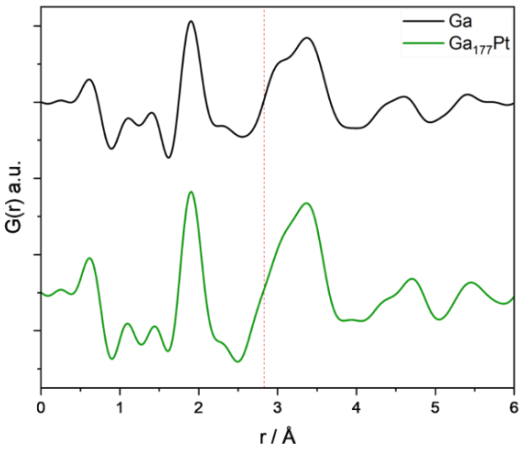

Figure 1: dPDFs of as-synthesized Pt-Ga SCALMS after subtraction of the SiO_2 support. The red dashed line highlights the contribution of the liquid phase to the dPDF [3].

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Probing the local lithium environment in Li-rich and Mn-rich disordered rocksalt materials for battery applications: a combined neutron and X-ray Pair Distribution Function study

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Keywords Disorder, PDF, Oxyde, Oxyfluoride, Modelling

Abstract

Lithium-rich compounds of the general formula $Li_{1+x}(M,M')_{1-x}(O,F)_2$ (where M and M' are transition metals, x> 0) exhibiting a disordered rock-salt structure have been of great interest to the battery community for about a decade. A representation of this type of structure is shown in Figure 1. When used as positive electrode materials in lithium-ion batteries, these compounds achieve stable specific capacities approaching 175 mAh/g while being free of critical elements such as cobalt and nickel, making them very attractive for use in electric vehicles. [1] These compounds are generally metastable, especially when containing significant amounts of fluorine, and are obtained by synthesis methods that “freeze” the cationic and anionic disorder (high temperature synthesis followed by quenching, mechanosynthesis, microwave heating synthesis, etc.).

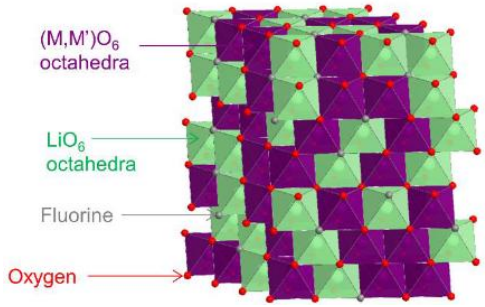

Figure 1. Three-dimensional representation of a disordered rocksalt structure

Therefore, a simple average rock-salt structure frequently does not capture the true local (dis)order, which is often considerably more complicated. Accurate descriptions of both local and average long-range structure in these materials are critical for any detailed understanding of the transport mechanisms and electrochemical performance.

In this context, the $Li_{1.25}Mn_{0.5+y/2}Nb_{0.25-y/2}O_{2-y}F_y$ (LMNOF) system with a rock-salt type structure is studied, and particularly two compounds: the parent oxide $Li_{1.25}Mn_{0.5}Nb_{0.25}O_2$, and the oxyfluoride $Li_{1.25}Mn_{0.7}Nb_{0.05}O_{1.6}F_{0.4}$. These two compounds were selected to investigate the impact of fluorine on the local structure of these materials and, consequently, on the pathways of lithium deintercalation and reintercalation. PDF is a valuable tool to investigate the local structure because it gives access to distances between ion pairs in the structure. Neutron PDF data is valuable to get information on Li while X rays PDF data gives us information on Mn and Nb in the structure. Combining both in a joint analysis using big box modelling with RMCProfile [2] provides a full picture of the local structure in the LMNOF materials.

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Structural Constraints for Complete Photonic Band Gaps in Quasiperiodic Dielectric Structures

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We investigate structural conditions underlying complete photonic band gap (CPBG) formation in two-dimensional quasiperiodic dielectric systems, aiming to bridge forward modeling and inverse design of aperiodic materials. Using quasiperiodic tiling approximants, including the Ammann–Beenker (8-fold) [1,2], square–triangle (12-fold) [3], and hexagon–boat–star (HBS) tilings (10-fold), we construct dielectric structures by placing air cylinders at the vertices of prototiles and compute TE and TM photonic band structures using the plane-wave expansion method.

It is confirmed that complete photonic band gaps appear in the square–triangle and HBS tilings, including the first CPBG reported for a quasiperiodic structure with 10-fold rotational symmetry. By introducing secondary air cylinders at the centers of star prototiles, the point density is systematically increased, resulting in the emergence of a CPBG in the Ammann–Beenker tiling and a substantial enhancement of the gap width in the HBS case.

To characterize the structural origin of gap formation, we analyze the systems in terms of hyperuniformity [4] and geometric complexity. In particular, the small-wavenumber behavior of the structure factor S(q) serves as an indicator of suppressed long-range density fluctuations relevant to isotropic gap formation [5]. Our results suggest that high point density together with reduced local structural complexity plays a key role in stabilizing complete photonic band gaps in quasiperiodic systems [6].

These findings provide insight into structure–property relationships in nonperiodic photonic materials and suggest possible structural descriptors for inverse design of aperiodic dielectric media.

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How does high pressure alter the hydrogen-bonded network in liquid methanol-water mixtures?

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Liquid methanol-water mixtures are good examples of the transition from a nearly fully connected single-cluster hydrogen-bonded (HB) system (in the water-rich region) to a more fragmented system containing chain-like clusters (in the methanol-rich region). It is already known that temperature influences the behaviour of the HB network under ambient conditions[1], so the question is whether it is influenced by pressure. In order to answer this question, a series of neutron diffraction (at the BL11 PLANET beam line in J-PARC MLF) [2], as well as energy-dispersive X-ray diffraction (at the BL04B1 beam line in SPring-8) experiments have been carried out. On the simulation side, classical molecular dynamics simulations have been performed. Considering the evaluation of energy-dispersive X-ray diffraction data, an evaluation procedure, inspired by [3], was developed and implemented. Although agreements of the molecular-dynamics simulated structure factors to the experimental datasets are only satisfactory, they follow the same trend. Based on the simulations, the network structure, based on the distributions of hydrogen bonded rings and chains will be presented.

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Molecular RMC modeling on combined data sets and a showcase of XRD software package A2D2

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This work is twofold in it's scope. First and most straightforwardly it utilizes the possibilities the molecular variant of the RMC-POT implementation offers by broadening it's employment both in regard to sample and probe. This treatise is flanked by a brief showcase on the XRD data analysis software package A2D2, highlighting it's fine control on data treatment especially alongside an evolving RMC analysis.

Building on the groundwork of Klee et al.[1], who implemented the handling and moving algorithms for molecules in the RMC-POT software package and first demonstrated it's practical value on the basis of X-ray diffraction data from the white-light-generating cluster molecule [(PhSn)4S6], the focus now shifts toward combining data sets of complementary probes, e.g. neutron diffraction, EXAFS spectroscopy as well as X-ray diffraction. This of course aims to further constrain and guide the RMC algorithm toward the physical qualities inherent to the respective sample. A demonstration for a pair of these sulfur-based clusters has been published by Pilgrim et al.[2]. Speaking of samples, the herein investigated molecules also originate from the growing library of white-light-generating cluster compounds, differing only in it's chemical composition from the cluster(s) examined by Klee and coworkers but retaining a predominantly similar molecular structure. The goal of the current work is to determine whether the intra-molecular distortions found by Klee et al. in the amorphous phase of [(PhSn)4S6] translate to similar clusters such as [(NpSn)4Se6] and [(MeSn)4Se6] sporting a modified cluster core (Selenium instead of Sulfur) as well as a different organic ligand sphere.

Furthermore the bespoken software package A2D2[3] is an in-house development of ours, capable of analyzing both total and anomalous scattering data. It provides various data correction steps that can be hand tweaked to suit disordered materials' scattering data and achieve cleanest possible X-ray S(Q)s for RMC use.

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Pair potential from force distribution and corresponding configurations

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The appearance of Reverse Monte Carlo simulation was interesting not only for experimental scientists, but it renewed the momentum on the theoretical field of the inverse theorem of statistical mechanics. More precisely, RMC initiated several methods, where pair interactions were determined from structural data. Later, it was extended with other methods, where energetic and dynamic data were used as input. The methods have got reasonable interest in the field of coarse graining in the last decade [1].

Theoretically, there are two equipartition theories in statistical mechanics [2]. The well-known one is the equipartition of the kinetic energy on the degrees of freedom and it is connected to the general and system independent kinetic energy and velocity distribution of the particles. The equipartition concerning the forces is less known, and no one was interested the provided distributions that are system dependent. In order to increase the variability of inputs of potential determination, we developed a method, where the inputs are force distributions and the corresponding configurations.

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Resolving local structural influences in quasi-linear dielectric, $NaNbO_3$-based systems using total scattering techniques

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Multilayer ceramic capacitors based on $NaNbO_3$-related perovskites are of significant interest for high power and voltage devices in energy storage applications. Recently, we designed the novel perovskite $0.88NaNb_{0.9}Ta_{0.1}O_3$–$0.1SrTiO_3$–$0.02La(Mg_{0.5}Ti_{0.5})O_3$ ($NNTa_{0.1}$–10ST–2LMT) which adopts a quasi-linear dielectric (QLD) state: one that exhibits a quasi-linear polarisation-electric field response, and exceptionally large energy density and permittivity maintained up to large applied fields.[1] These favourable properties, and hence the composition $NNTa_{0.1}$–10ST–2LMT, are therefore highly desirable for integration in real devices for high power applications.

From a crystallographic view, sequentially adding each component to $NaNbO_3$ has profound effects: $SrTiO_3$ stabilises the formation of a ferroelectric state with long range polar domains. $La(Mg_{0.5}Ti_{0.5})O_3$ suppresses long range polar coupling to form a weakly coupled relaxor state composed of polar nanoregions. Finally, Ta further reduces polar and structural correlation lengths to a few unit cells, reducing the *B* site polarisability and ultimately producing the desired QLD state. From this, the reduced degree of long range polar and structural coupling will have a profound influence on the average and local structures exhibited by these materials with increased compositional complexity. Therefore, in order to understand the emergence of the QLD state in $NNTa_{0.1}$–10ST–2LMT, it is essential to probe the structure-property relationships of these series of materials, especially in the local structure due to the incremental addition of each component to $NaNbO_3$.

This work presents preliminary Reverse Monte Carlo analysis using total scattering techniques to elucidate the local structural mechanisms underpinning QLD behaviour in $NaNbO_3$-based materials. The signatures we probe include correlated cation (*A* and *B* site) displacements and length scales of BO_6 octahedral tilting distortions. Challenges in the data analysis of these compositionally complex materials will be demonstrated, along with future directions in which these could be resolved, including the use of multi-dataset refinement approaches with other local structure probes.

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Water hydration at high pressure in Cu^{2+} solutions probed by x-ray absorption fine structure

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The hydration structure of aqueous Cu^{2+} ions remains controversial even under ambient conditions, and little is known under high pressure due to experimental limitations. In this study, the local structure of Cu^{2+} in aqueous solution was investigated in the pressure range 0.05-1.2 GPa using extended x-ray absorption fine structure (EXAFS) combined with reverse Monte Carlo (RMC) simulations. EXAFS spectra were analyzed using the GNXAS multiple-scattering approach.

The results show that the hydration structure is best described by a fivefold square-pyramidal geometry [2]. With increasing pressure, the axial Cu-O distance decreases while the equatorial Cu-O distances slightly increase. RMC analysis confirms these trends at the distribution level and further reveals narrowing of the O-Cu-O angle distribution, indicating reduced angular disorder under pressure.

These results show that pressure slightly reduces the structural anisotropy of the fivefold coordination environment without changing the coordination number.

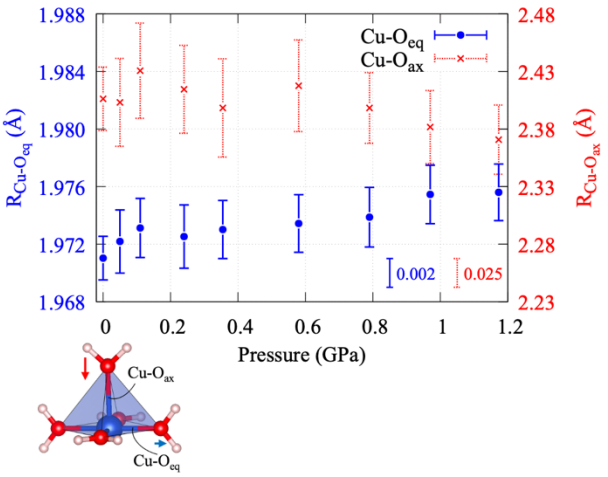

Figure 1. Pressure dependence of the distances for Cu-O_{eq} (left axis, solid line) and Cu-O_{ax} (right axis, dashed line) in the Cu^{2+} solution by EXAFS analysis.

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Probing ZnO Lattice Dynamics via EXAFS and Reverse Monte Carlo Modeling

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In this study, extended X-ray absorption fine structure (EXAFS) spectroscopy was employed to probe the temperature-dependent local lattice dynamics of polycrystalline wurtzite-type ZnO, which crystallizes in a hexagonal lattice ($P6_3mc$) with tetrahedral Zn–O coordination. Experimental Zn K-edge EXAFS spectra [1] were collected over the temperature range 300-1200 K in transmission mode at the BALDER beamline of the MAX IV Laboratory [2]. The reverse Monte Carlo (RMC) method, combined with an evolutionary algorithm [3], was used to obtain the Zn–O and Zn–Zn radial distribution functions (RDFs), including contributions from coordination shells up to 7 Å. The RDFs were decomposed into Gaussian peaks to extract the mean-square relative displacements (MSRDs) for Zn–O and Zn–Zn coordination shells. Effective force constants, describing the stiffness of interatomic interactions, were derived from the temperature dependence of the MSRDs for each shell using the Einstein model [3]. The results were compared with those from conventional data analysis for the first two coordination shells, as well as with previously reported low-temperature data [4]. The atomic motion of the Zn–O pair is strongly correlated due to the strength of the interatomic bond, and this correlation increases with temperature.

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The structure of GeO_2 from glass to melt: Can RMC shed some new light?

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Glasses are ubiquitous in both nature and technology [1]. They are the oldest synthetic materials produced by humans and contributed to shaping the world as we know it, to the point that it has been proposed that we are now living in the *Glass Age* [2]. Despite this, a global theory of the glassy state is still lacking, and structural studies remain essential to uncover the microscopic origin of their unique properties.

Here, we investigate the structural evolution with temperature of glassy GeO_2, a prototypical strong glass-former and network-forming system [3]. Time-resolved isothermal neutron total scattering data were collected at different temperatures between the glass and the liquid. The evolution of the total structure factor *S(Q)* and the corresponding total radial distribution function *G(r)*, reveals subtle structural changes with temperature as well as structural relaxation near the glass transition. However, for a multi-component system such as GeO_2, these observables provide mainly indirect and largely qualitative information.

To obtain a quantitative, real-space description of these changes, we aim to employ Reverse Monte Carlo (RMC) modeling. The initial configuration will be generated by a molecular dynamics melt-quenching simulation using the well-established Oeffner-Elliott potential [4] and then refined against the experimental data at room temperature. This refined structure will then serve as the starting point for refinement at the next temperature, enabling an iterative procedure tracking the structural evolution from the glass up to the liquid.

Preliminary tests indicate that the neutron data alone are insufficient to constrain the algorithm robustly, motivating a complementary X-ray total scattering experiment. A key experimental challenge is the X-ray induced dynamics and the associated amorphous-amorphous transformation [5], a well-documented effect for oxide glasses at third generations synchrotron sources. Then, the experiment will be optimized to collect data representative of the pristine structure. Subsequently, controlled irradiation will be used to characterize the beam-induced structural evolution itself, providing its first quantitative real-space description.

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