

Seeing Beyond Crystallography

*Pair Distribution Function Analysis of Complex Materials
— from the laboratory diffractometer to the spallation source —*

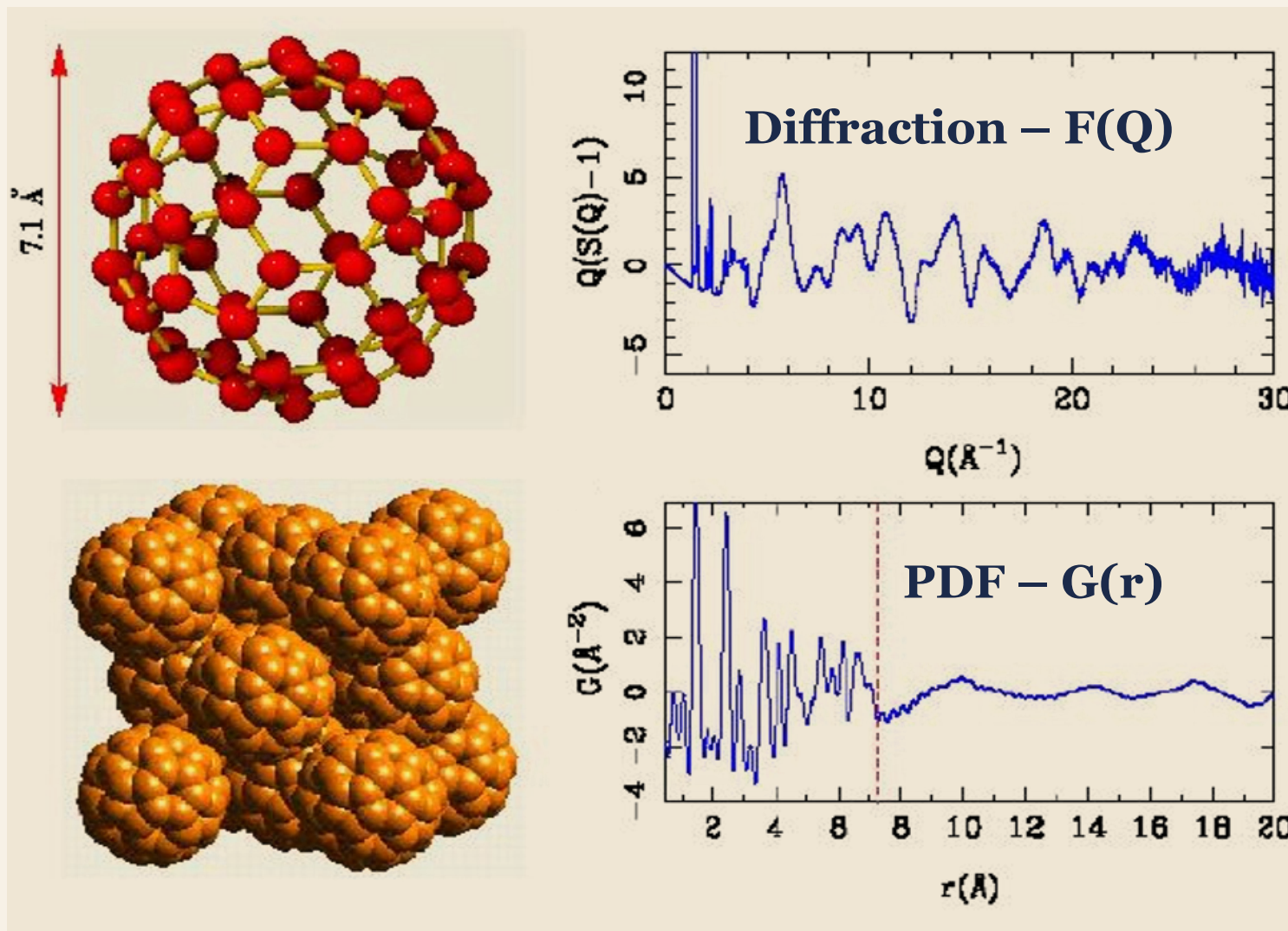
Emil S. Bozin
Institute of Physics Belgrade



28 September 2026 · 16:30 · 45 min · Lecture Hall, CC Academia

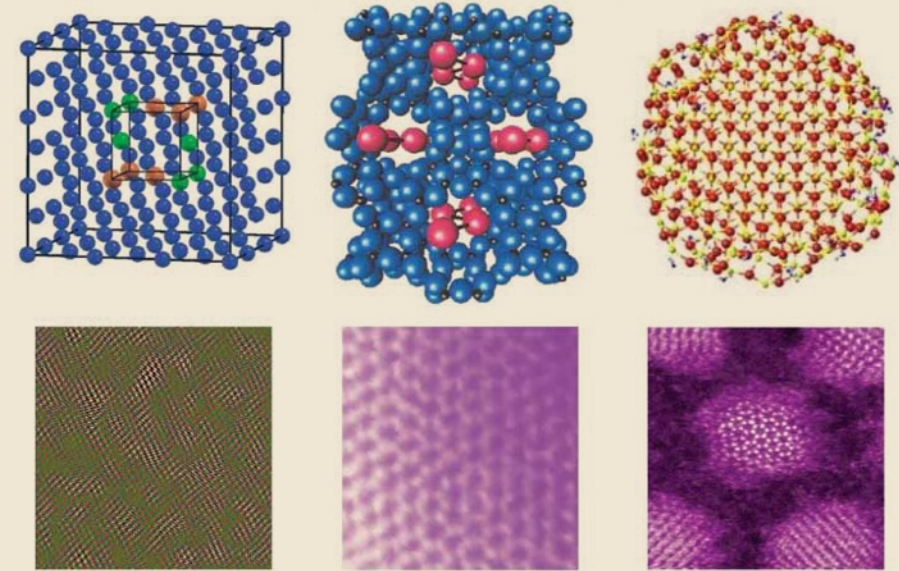


PDF primer: The case of C_{60}



PDF scope: Hierarchy of structure length-scales in materials

- Non crystalline materials
(liquids, amorphous solids, polymers)
- Nanoscale materials
- Disordered crystalline systems
with nanoscale heterogeneities

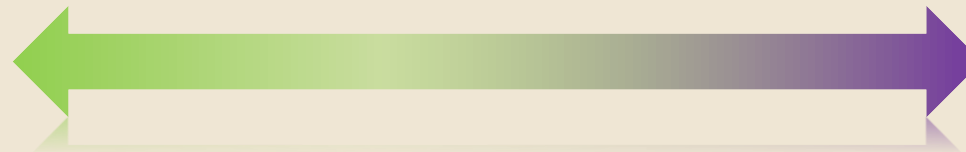


S.J.L. Billinge and I. Levin, **The Problem with Determining Atomic Structure at the Nanoscale**, *Science* **316**, 561 (2007).

molecule



crystal



Forty minutes, five arguments

01 Why the average structure is not (always) the structure

02 What $G(r)$ actually is — and what it is not

03 Three sources: lab XRD, synchrotron, spallation neutrons

04 How the experiment and the model can deceive

05 Case studies with references you can open tonight

01

Why the average structure is not the structure

The average crystal structure often masks the underlying structural heterogeneity that defines the material's true complexity.

The slide crystallographers cannot show you

A material can be cubic on average and orthorhombic in every unit cell. A battery cathode can look single-phase by Rietveld and two-phase by PDF. A 3 nm particle can have a well-defined core structure and no usable Bragg pattern.

The illusion of the average

Bragg intensities are the **periodic projection**. Local distortions, stacking faults and nano-domains are averaged into ADPs or thrown into the background.

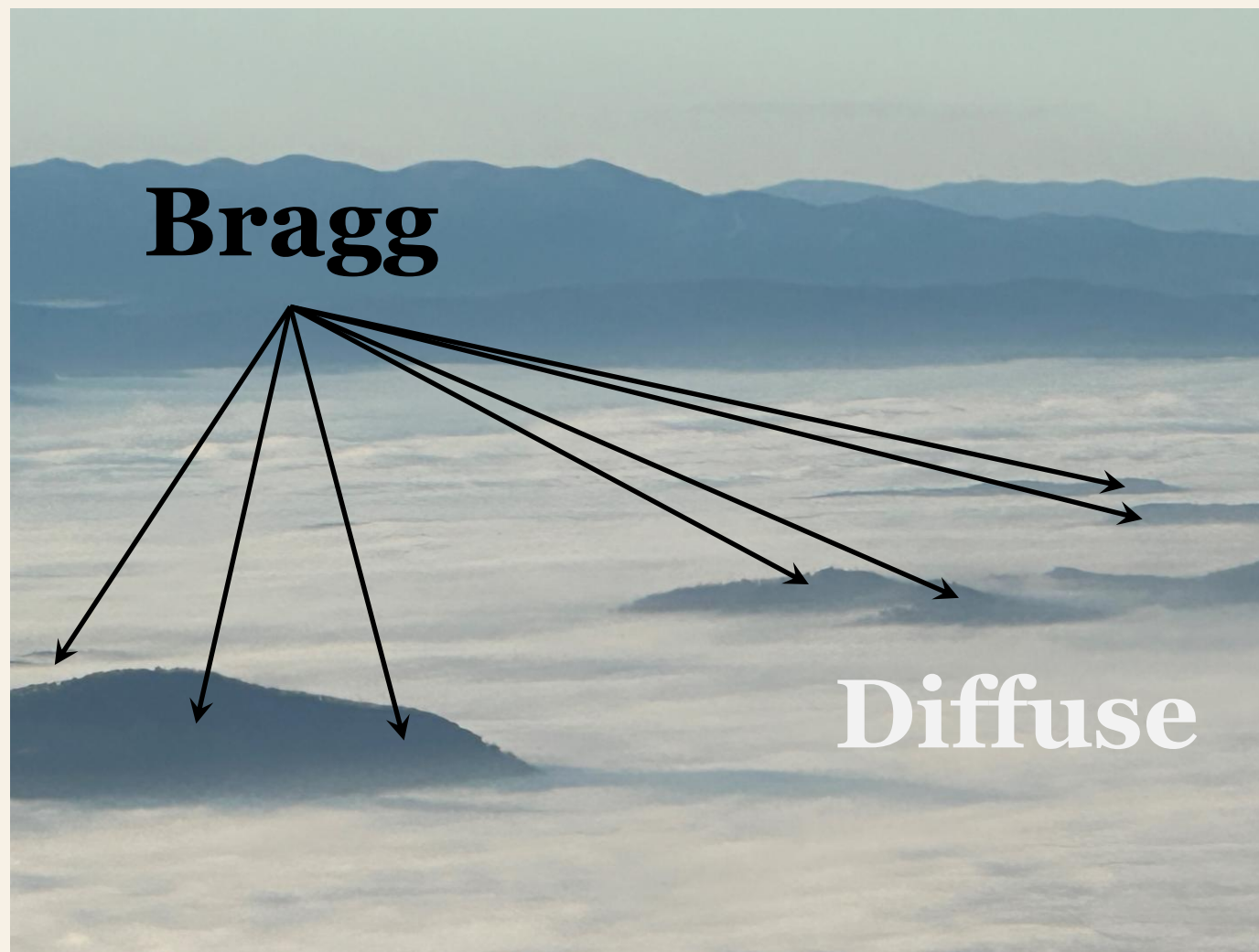
The missing intensity

Diffuse scattering between the peaks **is not noise**. It is the pair correlations that do not repeat.

The real-space move

Fourier-transform the whole pattern. The result is **PDF**, $G(r)$, a **weighted histogram of every interatomic distance** in a material.

The PDF approach: Diffuse scattering on par with Bragg



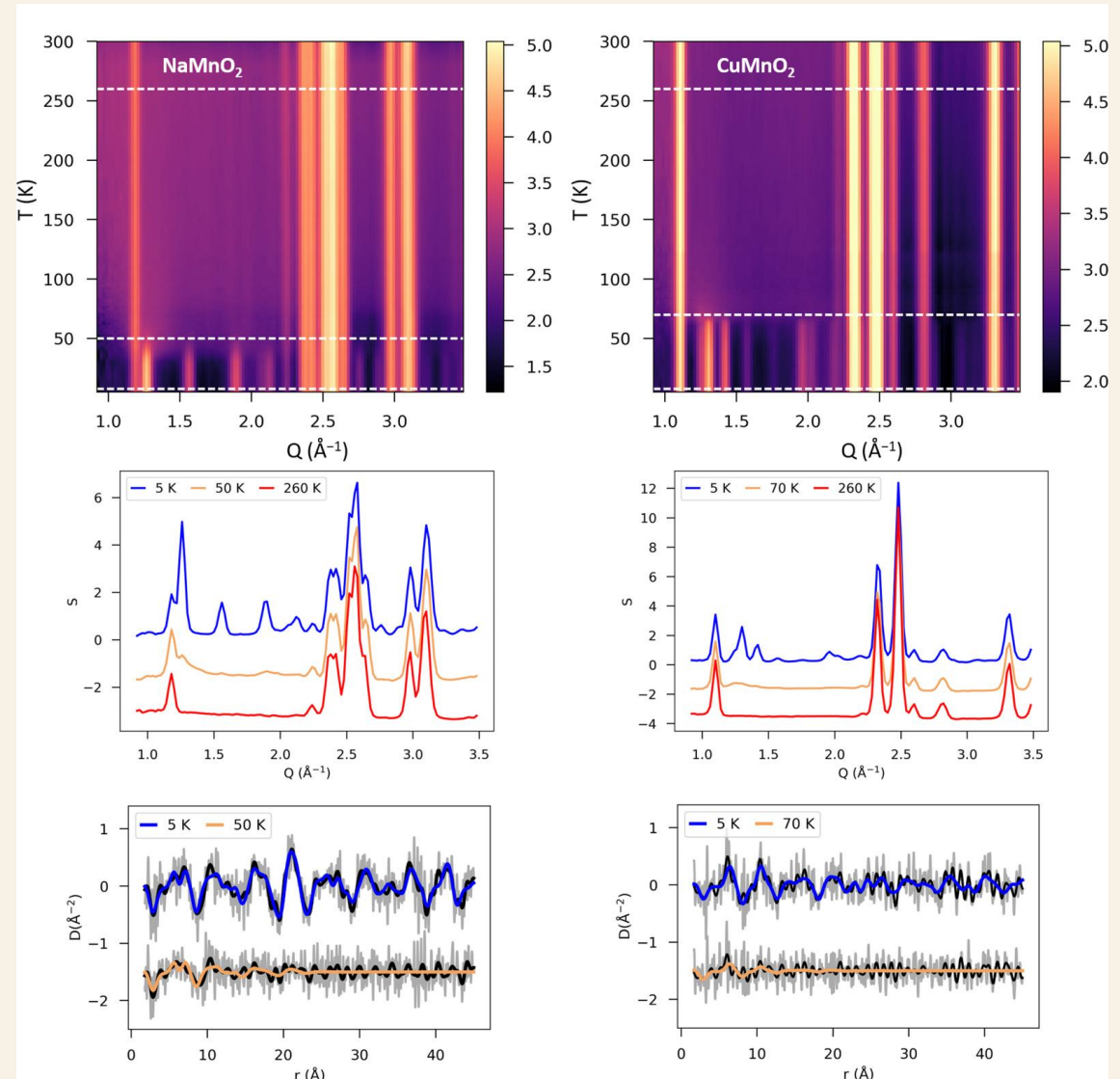
Illustrative example: Magnetic diffuse scattering @ $T > T_N$

Diffuse signal is often **delicate**, spread throughout Q-space, but **it is there!**

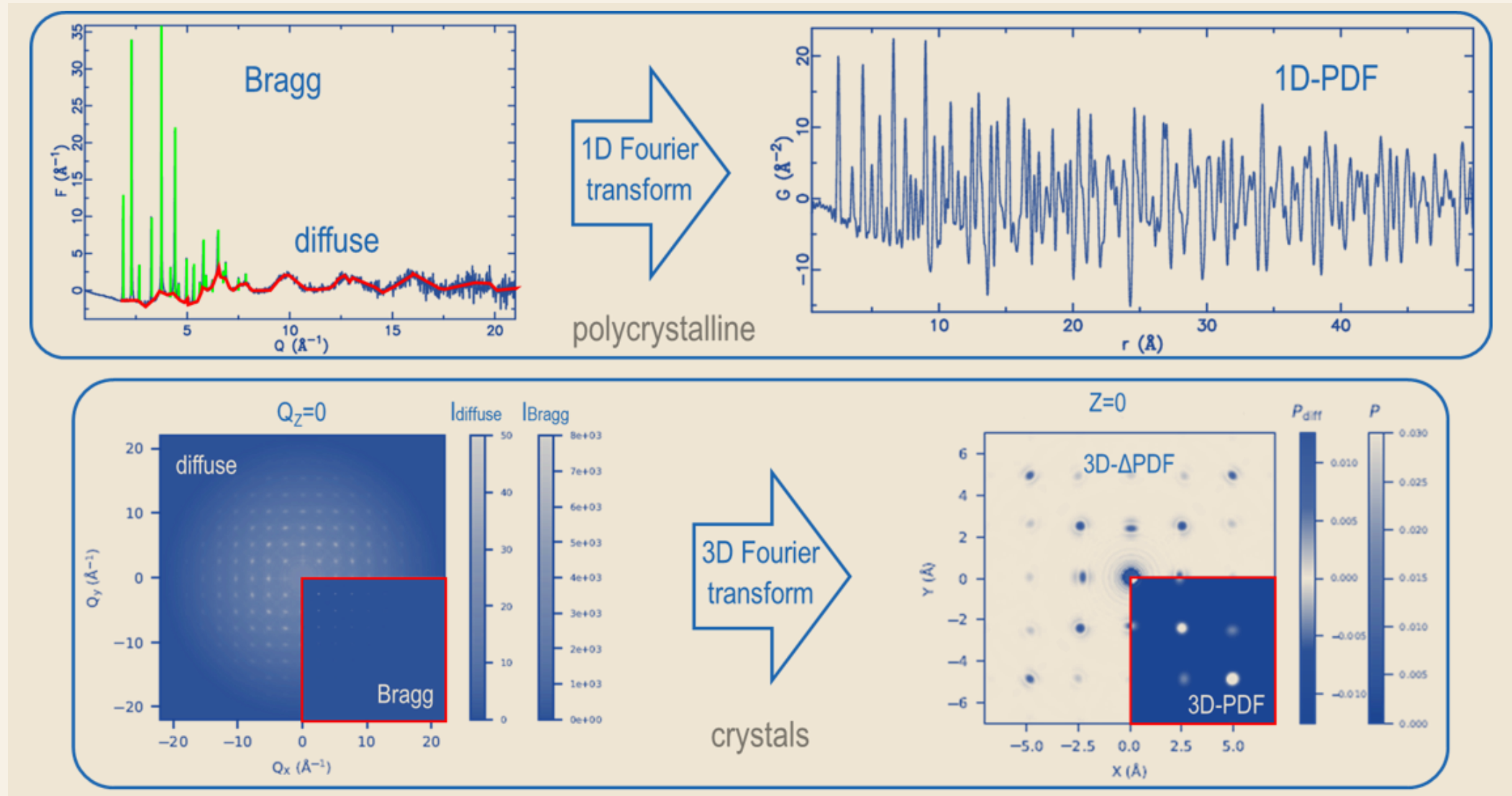
T-swipe

Selected T-cuts

mPDF

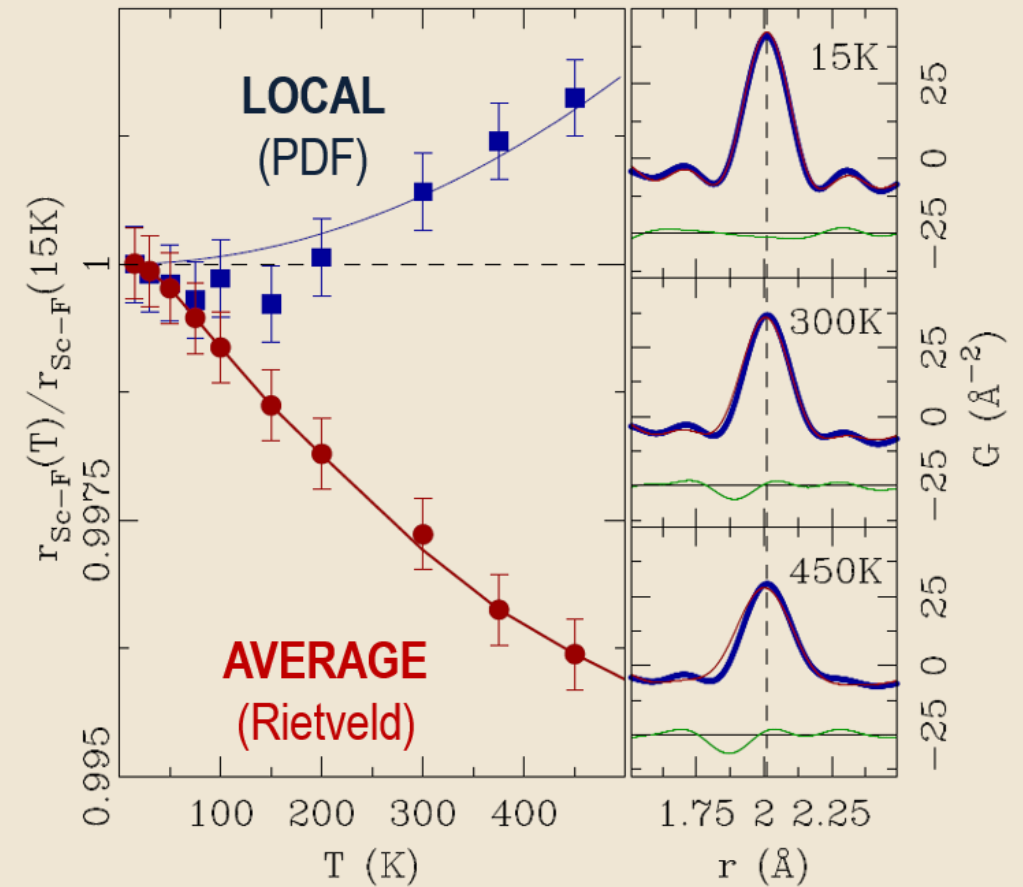
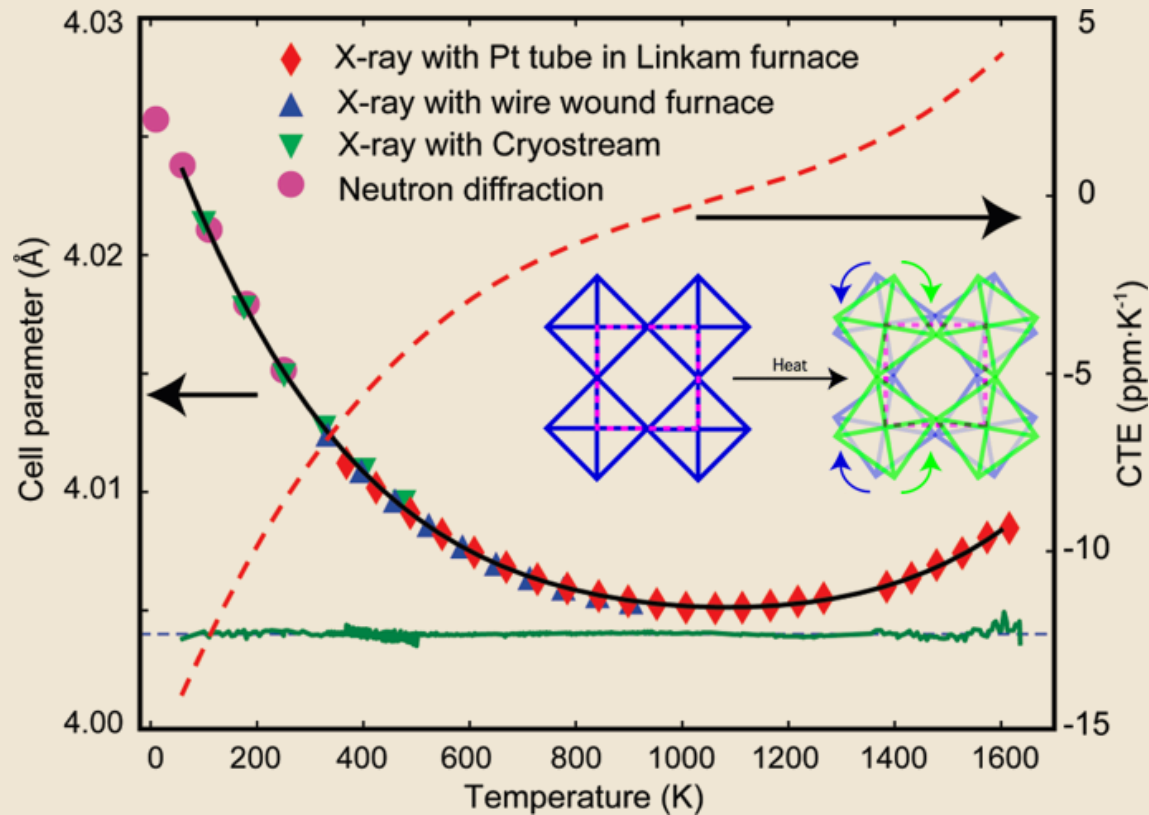


Advanced Fourier maps: The pair distribution function approach



R.J. Koch et al. *Acta Cryst. A* 77, 611–636 (2021)

Illustrative example: Huge negative thermal expansion in ScF_3

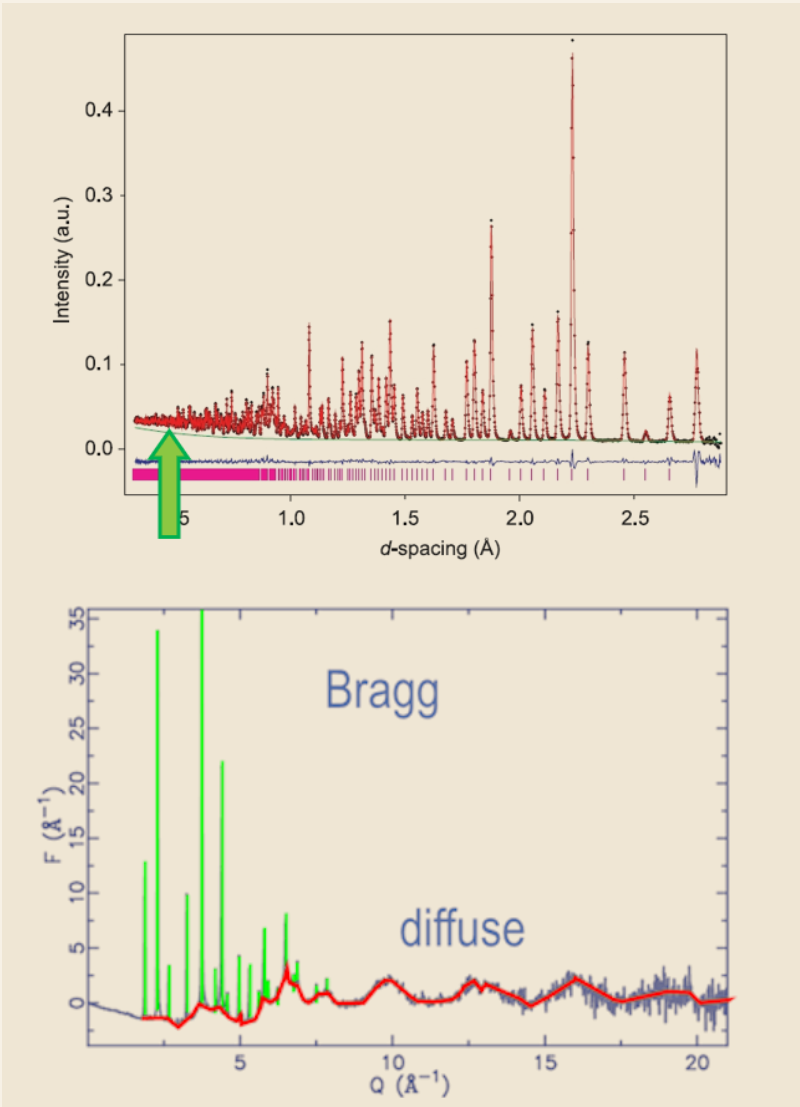


What a Rietveld refinement allows you to know

Observable	Bragg / Rietveld	Lost unless you keep the diffuse intensity
Periodicity	Space group, lattice, long-range order parameter	Finite correlation length, nano-domains
Positions	Wyckoff sites of the average cell	Split sites, off-centering, stacking faults
Chemistry	Site occupancies as space–time averages	Chemical short-range order, clustering
Motion	ADPs = static + dynamic, uncorrelated by construction	Correlated displacements, polarons, rattling
Size	Scherrer width — a reciprocal-space smear	Real-space envelope of $G(r)$

Egami & Billinge, Underneath the Bragg Peaks (Pergamon/Elsevier, 2003; 2nd ed. 2012). Billinge & Levin, Science 316, 561 (2007).

Keep the stuff between the peaks!



Rietveld fit

Models the Bragg peaks. Treats the slowly varying intensity as background. **That background is often the physics!**

Total scattering

Normalize the entire pattern to $S(Q)$. **Bragg and diffuse enter the same Fourier integral.** Nothing is optional.

Schematic after Egami & Billinge (2012), Ch. 3. Diffuse intensity is the Fourier transform of deviations from the average.

02

What $G(r)$ actually is — and what it is not

$G(r)$ reveals how atoms are arranged across length scales—not a unique structure, but a statistical picture of local atomic correlations.

The pair distribution function in one sentence

$$G(r) = (2/\pi) \int Q [S(Q) - 1] \sin(Q r) dQ$$

A signed, weighted histogram of interatomic distances. Positive (and sometimes negative) peaks: pairs in excess of the average density.

Position

Bond length. Jahn–Teller split. Off-centering.

Width

Uncorrelated static + dynamic disorder of that pair.

Area

Coordination × scattering contrast.

Range

How far the local order extends.

The pair distribution function in one sentence

$$G(r) = (2/\pi) \int Q [S(Q) - 1] \sin(Q r) dQ$$

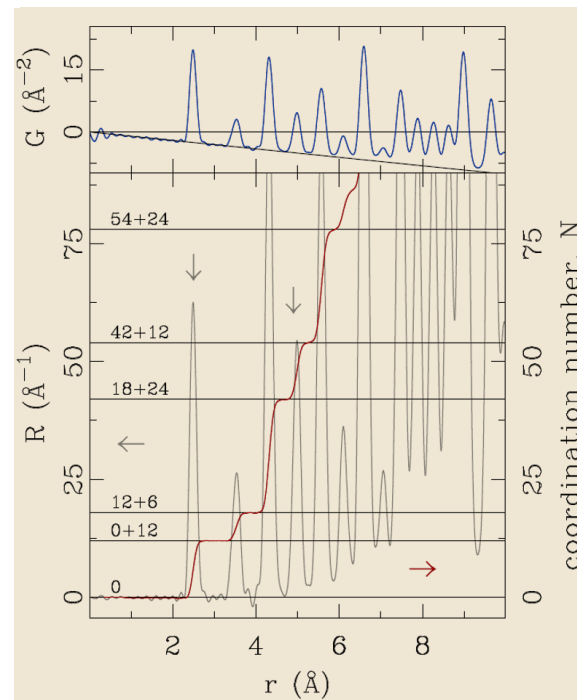
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Width

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Range

How far the local order extends.

PDF analysis concept & experimental cycle

$$I_{tot} = I_{sam} + I_{bgd}$$

$$I_{sam} = A \cdot P \cdot [C \cdot I_{coh} + I_{inc} + I_{mul}]$$

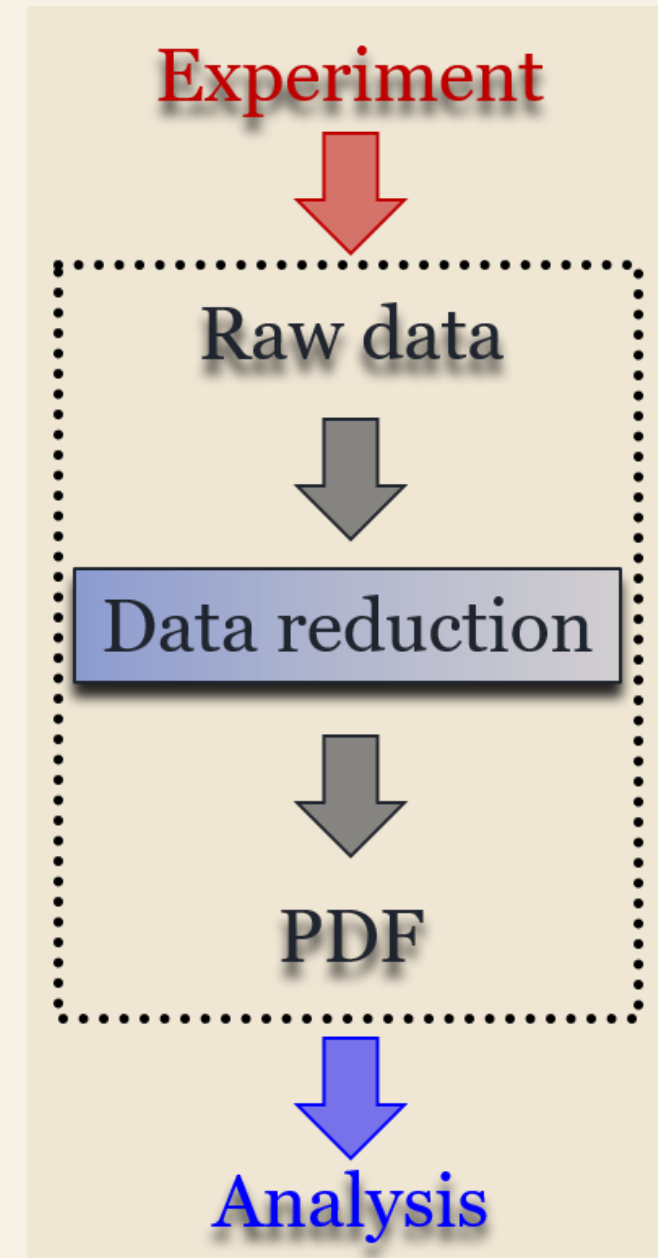
$$S(Q) = \frac{I_{coh}(Q) - \langle b^2 \rangle + \langle b \rangle^2}{\langle b \rangle^2} \quad Q = \frac{4\pi \sin \theta}{\lambda}$$

$$G(r) = \frac{2}{\pi} \int_0^{\infty} Q (S(Q) - 1) \sin Qr \, dQ$$

$$G(r) = \frac{1}{Nr \langle b \rangle^2} \sum_{i \neq j} b_i b_j \delta(r - r_{ij}) - 4\pi r \rho_0$$

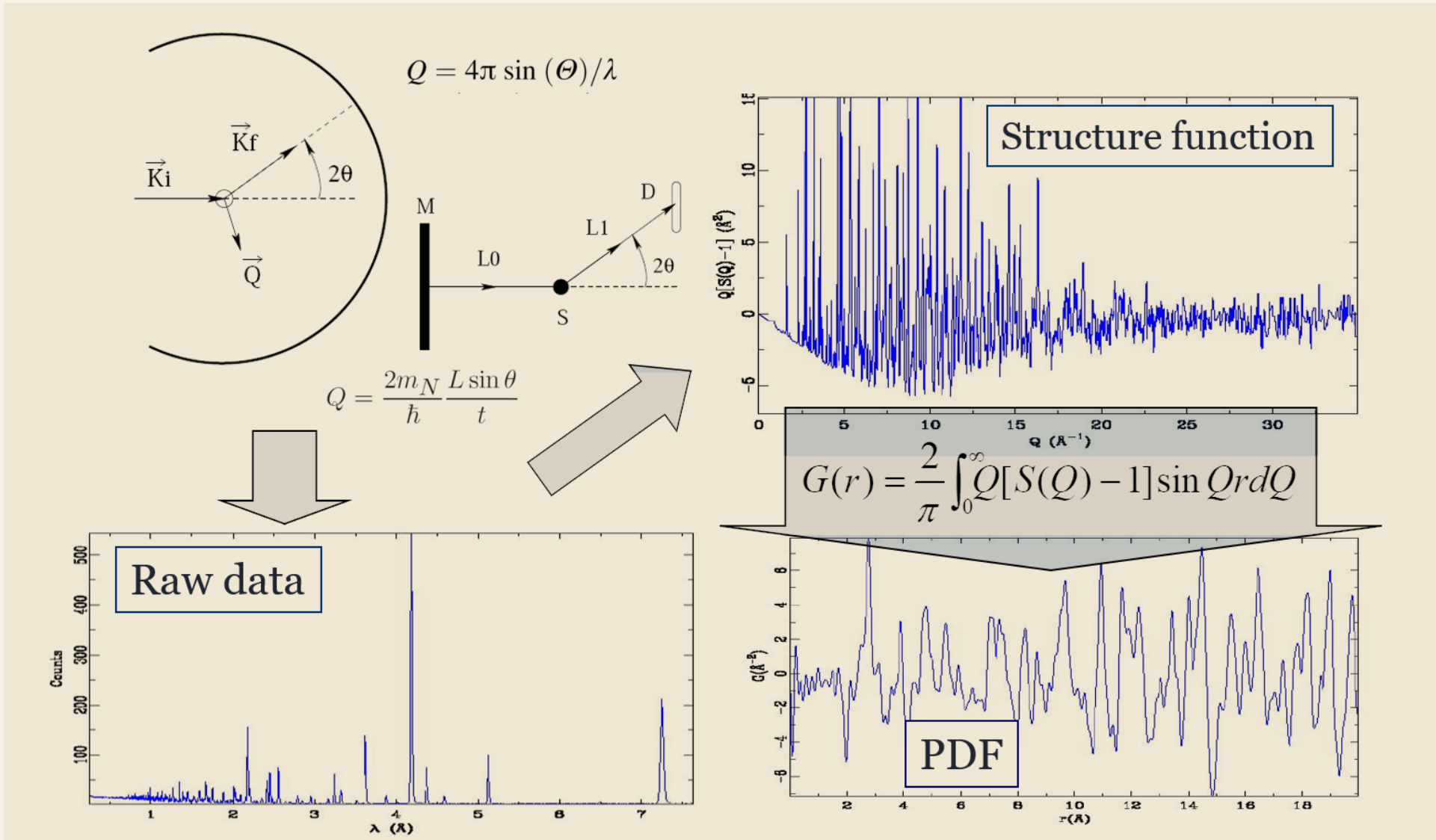
Experiment

Model



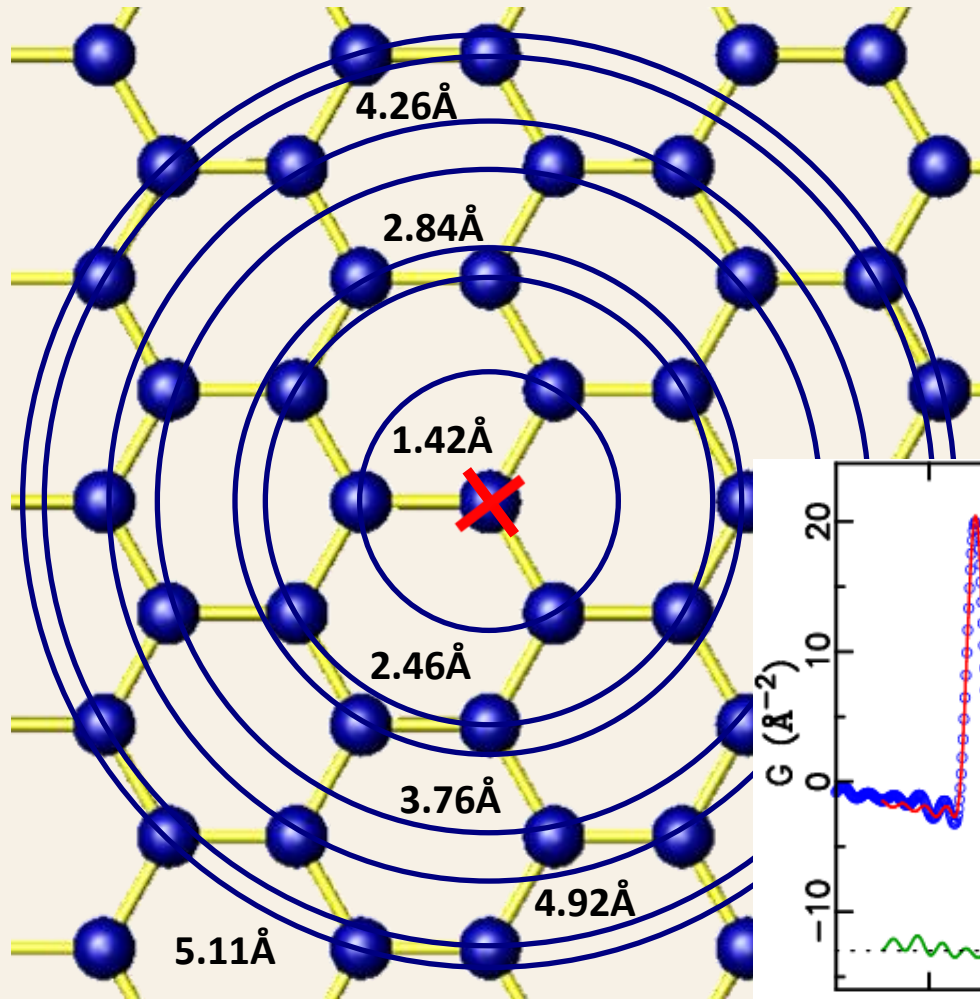
From Egami & Billinge (2012).

Visual overview of PDF cycle & methodology

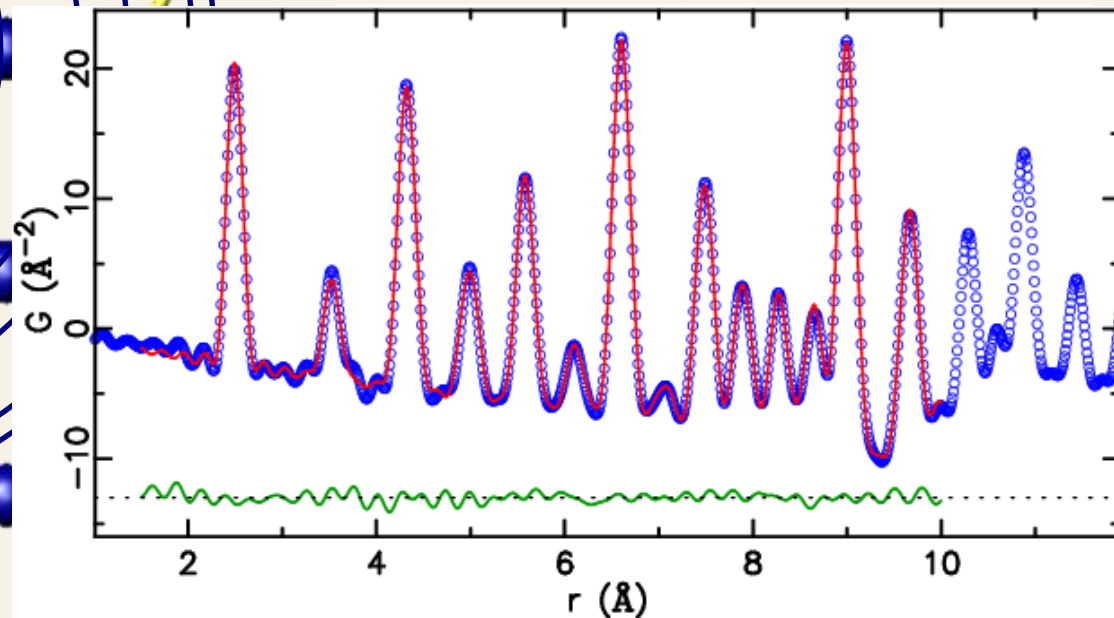


From Egami & Billinge (2012).

Read $G(r)$ like a radial crystal – Real-space pair-distance histogram

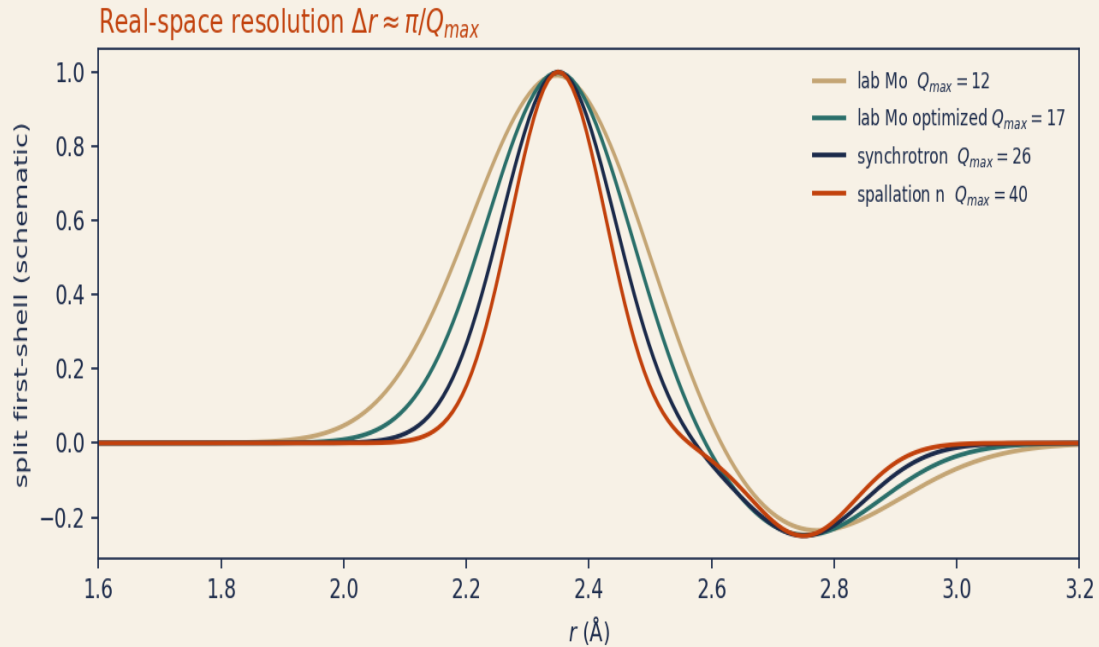


Radial atomic **pair** distribution function (PDF) gives the inter-atomic distance distribution, or “probability” of finding atomic pairs distance r apart



Textbook description as in Egami & Billinge (2012).

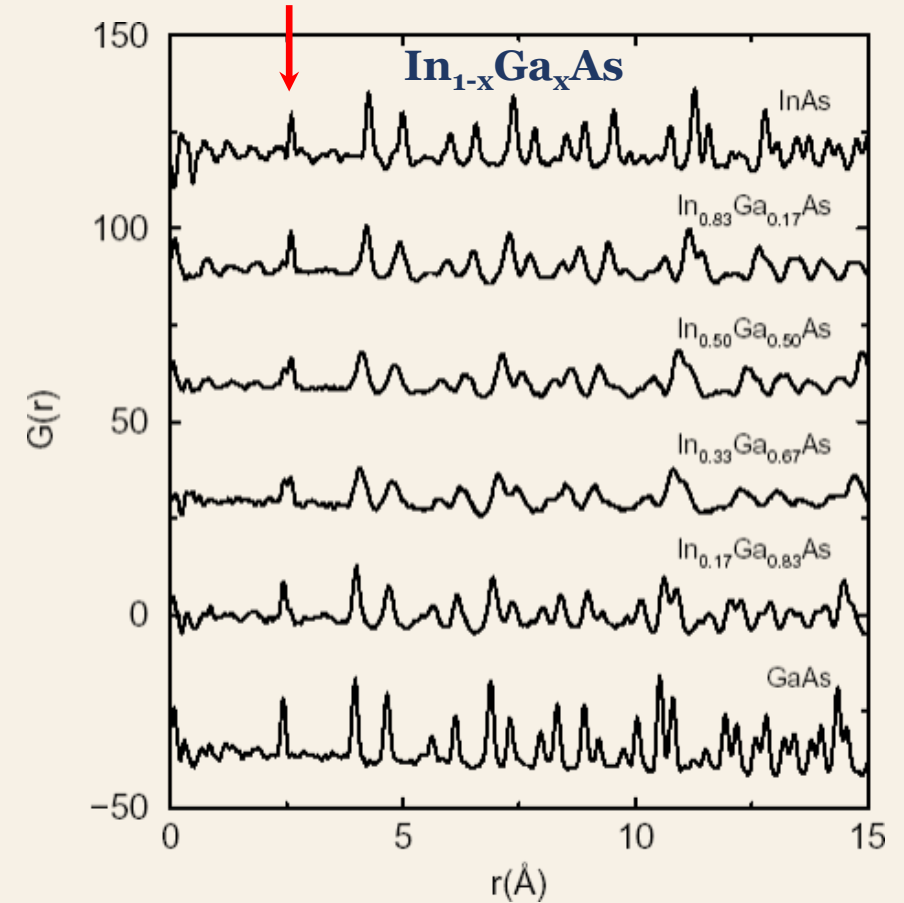
Q_{MAX} is not a detail. It is the resolution.



Lab Mo K α — $Q_{\text{max}} \approx 12\text{--}17 \text{ \AA}^{-1}$. First-shell splitting of $\sim 0.2 \text{ \AA}$ is painful.

Synchrotron 60–80 keV — $Q_{\text{max}} \approx 25\text{--}30 \text{ \AA}^{-1}$ routine. Split bonds become peaks.

Spallation neutrons — $Q_{\text{max}} \approx 30\text{--}50 \text{ \AA}^{-1}$. Form factor does not die. Best raw resolution.



$$G(r) = \frac{2}{\pi} \int_{Q_{\text{MIN}}}^{Q_{\text{MAX}}} Q (S(Q) - 1) \sin Qr \, dQ$$

$\Delta r \approx \pi/Q_{\text{max}}$. High- Q tail of $S(Q)-1$ is small — that is exactly where resolution is bought. Egami & Billinge (2012), §3.2. I.-K. Jeong et al., Local structure study of $\text{In}_x\text{Ga}_{1-x}\text{As}$ semiconductor alloys using high energy synchrotron x-ray diffraction, Phys. Rev. B 63, 205202 (2001)

03

Three ways to buy a PDF

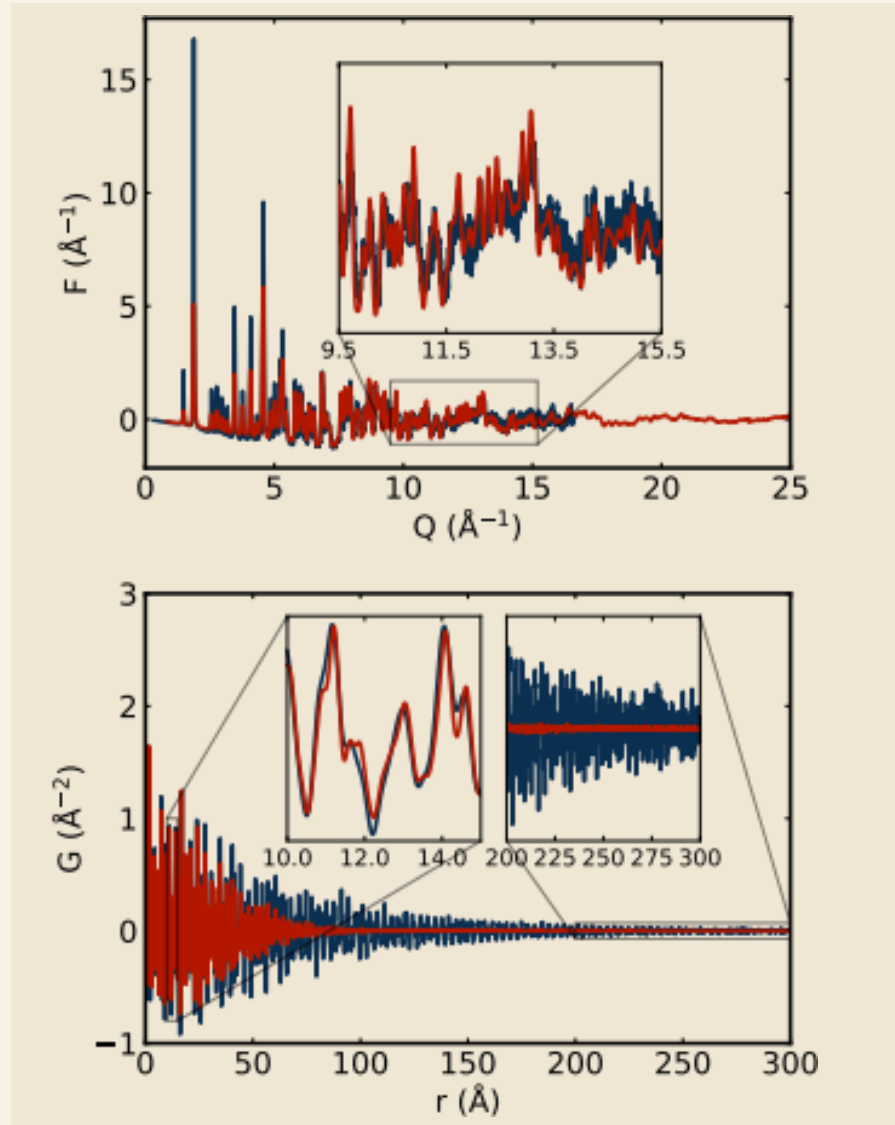
A laboratory Mo/Ag diffractometer, a high-energy synchrotron beamline, and a pulsed spallation neutron instrument **are not the same experiment!**

The comparison that should be on the wall

	Lab XRD (Mo/Ag)	Synchrotron XRD	Spallation neutrons
Q_{MAX}	12–17 (Mo) / ~22 (Ag) Å ⁻¹	25–30 Å ⁻¹ typical; 40 possible	30–50 Å ⁻¹
Time / pattern	overnight-days	seconds–minutes	minutes–hours
Sample mass	tens of mg	mg, even µg in capillaries	0.1–few grams
Light atoms	Poor next to heavy Z	Poor next to heavy Z	O, Li, N, D excellent
H / D	Almost invisible	Almost invisible	H incoherent; D coherent
Form factor	Falls with Q	Falls with Q	Flat (nuclear)
Access	Walk-up, screening	Proposal + beamtime	Proposal + beamtime
Killer app	Triage, teaching, coarse local order	Parametric, operando, nano	Oxygen networks, hydrides, mPDF

Compiled from Keen, J. *Appl. Cryst.* / reviews of neutron total scattering (2022); Schertenleib et al., *Chem. Methods* (2025); Egami & Billinge (2012).

In-house XRD PDF is real — if you earn the high-Q tail

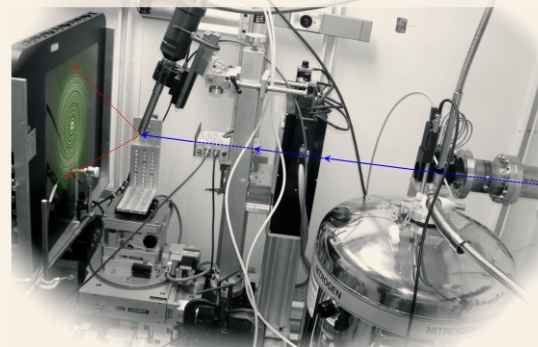


In-house Mo K α

Synchrotron RA-PDF



High data throughput PDF setup at X17A, NSLS, BNL



What the 2025 protocols showed

Mo K α , Bruker D8, staircase counting at high angle, Soller slits for crystals, absorption correction in PDFgetX3.

Quartz: lab $R_w \approx 0.15$ after 25 h vs synchrotron $R_w \approx 0.14$ in 15 min. Peaks overlay to $\sim 20\text{--}30$ $\text{\AA}$. ADPs inflate on the lab data.

Use the lab to decide whether a beamtime proposal is worth writing.

Numbers from the lab-versus-synchrotron benchmark

	NSLS-II 28-ID-1	Lab Mo, protocol P2
Wavelength	0.1665 Å (high-E)	0.7107 Å (Mo Kα)
Q _{MAX} used	26.0 Å ⁻¹	16.6 Å ⁻¹
Wall-clock	15 minutes	25.5 hours
a (Å)	4.916540(5)	4.91055(13)
c (Å)	5.409109(10)	5.40225(23)
R _w	0.137	0.147
O U ₁₁ (Å ²)	0.0214	0.0509 (inflated)

Schertenleib et al., Chem. Methods (2025). DiffPy-CMI fits of α-quartz, 1–40 Å.

Why the synchrotron still wins most PDF arguments

Hard X-rays

60–80 keV shrinks absorption, kills most fluorescence problems, and pushes 2θ coverage into $Q > 25 \text{ \AA}^{-1}$ on an area detector 20 cm away.

Minutes, not a day

A temperature, gas or electrochemical point costs as much as a coffee. Operando PDF is a synchrotron sport.

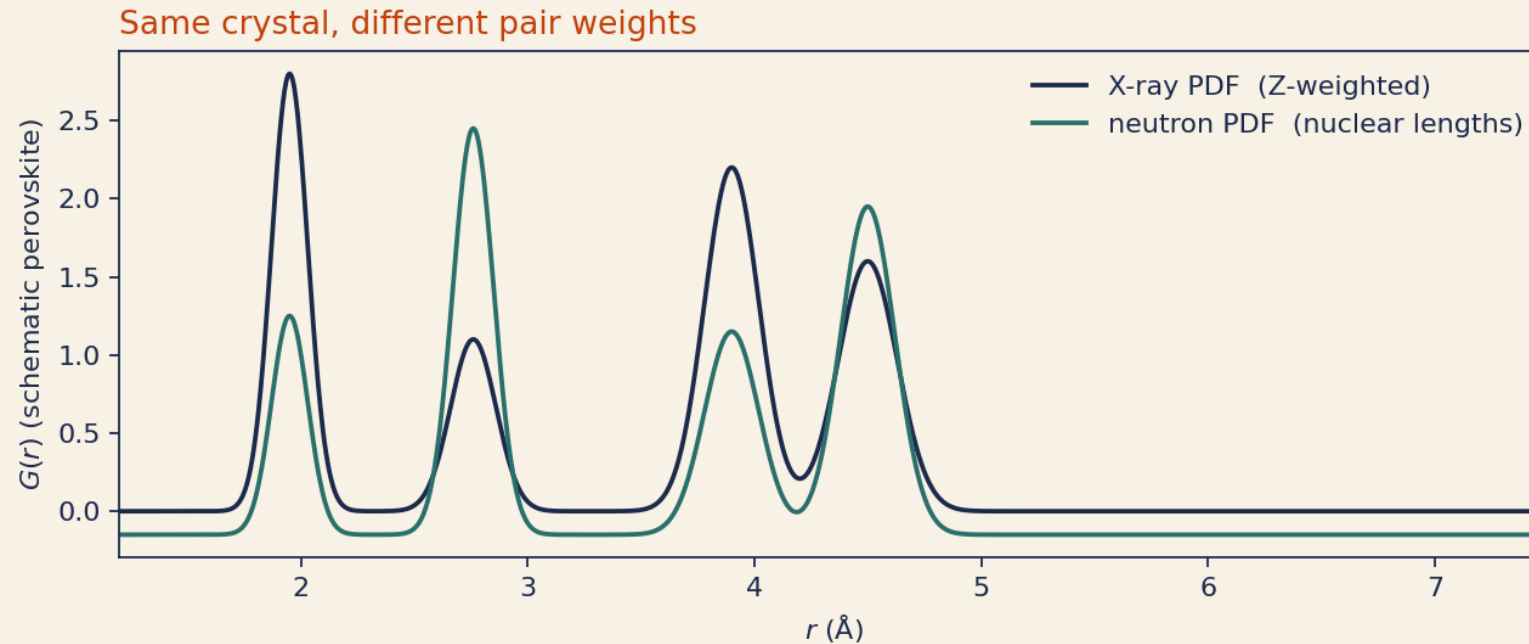
Small and nasty samples

Air-sensitive capillaries, thin coatings, 1 mm of a precious phase. Flux buys the high- Q tail you cannot count at home.

What it cannot do

See oxygen next to tungsten. Separate Mn from Fe. Give you a PDF tomorrow morning without a proposal.

Spallation neutrons: contrast, not just Q_{MAX} (...and magnetism)



- ▶ Nuclear lengths do not track Z . Oxygen is a first-class citizen. Li and N are visible. Neighbouring 3d metals can be told apart.
- ▶ b is Q -independent: the high- Q tail does not die of form factor. That is why neutron $G(r)$ can be sharper even at similar Q_{max} .
- ▶ Isotopic substitution (H/D , $^6\text{Li}/^7\text{Li}$, $^{58}\text{Ni}/^{60}\text{Ni}$) yields partial PDFs — something X-rays cannot buy with energy.
- ▶ Cost: grams of sample, incoherent H, Placzek inelasticity, vanadium cans, and a proposal.

NOMAD/POWGEN (SNS), GEM/POLARIS/NIMROD (ISIS), NOVA (J-PARC). Božin et al., *J. Appl. Cryst.* 42, 724 (2009) — ARCS PDF.

A brutally practical decision tree

You need to know...	Start here
Is there any local signal at all?	Lab Mo PDF overnight. If $G(r)$ is a ripple farm, fix the sample first.
Bond split $< 0.15 \text{ \AA}$, or a parametric movie?	Synchrotron. Do not pretend otherwise.
Where is the oxygen / lithium / vacancy?	Spallation neutrons. X-rays will flatter the cations.
Are two 3d metals ordered?	Neutrons, or resonant X-ray PDF if you must.
Nanoparticle in a capillary, 5 K points?	Synchrotron RAPDF. Lab will age you.
Magnetic correlations?	Magnetic neutron PDF (mPDF). Different Hamiltonian, same transform.
Tomorrow morning, teaching lab, screening 8 batches?	In-house. That is why the lab instrument exists.

Textbook description as in Egami & Billinge (2012).

04

How the experiment and the model can deceive

Experiments reveal only what we **measure**, and **models** only what we **assume**—both can conceal the structural reality beneath.

The measurement is won at high Q

Count the tail

$S(Q)-1$ at $Q = 20 \text{ \AA}^{-1}$ is tiny. If your detector is bored there, $G(r)$ will be a sine wave.

Empty everything

Capillary, air, windows. A 2% leftover container is a long-period baseline in $G(r)$.

Geometry is a systematic

Beam center, sample–detector distance, wavelength.
Calibrate on Ni or Si every run.

Q_{DAMP} is not size

Instrumental Q -resolution damps high- r . Measure it. Do not sell it as a 4 nm particle.

Reduction is not a button. It is a claim.

- | | | |
|----------|-----------------------------|---|
| 1 | Integrate | Mask beamstop, dead pixels, single-crystal spots from windows. |
| 2 | Subtract | Empty cell + air, scaled. Absorption and polarization. |
| 3 | Normalize | Divide by $\langle f(Q) \rangle^2$. Compton out. $S(Q) \rightarrow 1$ at high Q . |
| 4 | Transform | Choose Q_{MAX} , Q_{MIN} , optional window. Inspect low- r ripples. |
| 5 | Audit | Number density physical? First peak where chemistry says? Ripples move with Q_{max} ? |
| 6 | Publish the metadata | Q_{MAX} , Q_{DAMP} , Q_{BROAD} , r_{POLY} , container. Or the $G(r)$ is not reproducible. |

Inspired by Textbook of Egami & Billinge (2012).

X-rays vs neutrons: correction priorities differ

X-ray total scattering

- polarization
- photoelectric absorption / self-absorption
- Compton (incoherent) scattering
- fluorescence (especially at lower energies)
- detector efficiency / solid angle
- multiple scattering
- container + air background

Neutron total scattering

- detector efficiency / incident flux
- sample + container scattering
- absorption / attenuation
- multiple scattering
- incoherent scattering (including isotope-dependent terms)
- normalization, commonly against vanadium
- background / empty-container corrections

What is being corrected? Additive vs multiplicative effects

A useful mental model is:

$$I_{\text{TOT}}(Q) \approx P(Q) A(Q) D(Q) [I_{\text{COH}}(Q) + I_{\text{COMPTON}}(Q) + I_{\text{MULTIPLE}}(Q)] + I_{\text{BG}}(Q)$$

Additive contributions

container / air / sample environment
Compton or other unwanted components
fluorescence

Multiplicative contributions

absorption / attenuation
polarization
solid angle / detector response
flux / normalization

Geometry / instrumental

Q calibration
sample displacement
detector geometry / resolution

The exact factorization is instrument- and software-dependent; this equation is a bookkeeping representation, not a universal reduction formula!

Three levels of model, in the order you should climb them

0. Look

Peak positions, widths, areas, and the r at which oscillations die. Many papers should have stopped here and been better for it.

1. Small box

One unit cell + ADPs + occupancy + spherical envelope. PDFgui / DiffPy-CMI / TOPAS. Fast, named parameters, the correct first model.

2. Large box

RMC, EPSR, MD, 10^4 atoms. Use when one cell cannot tell the truth. Constrain hard or you will fit termination ripples.

How to publish a peak that does not exist

Termination ripples

Vary Q_{MAX} . Real peaks stay put; ripples march.

Wrong ρ_0

Tilts the baseline and invents coordination numbers.

Qdamp sold as size

Fit a standard in the same geometry first.

R_W worship

Split every site and R_W falls. Chemistry does not.

One RMC snapshot

An ensemble plus constraints is a result. A pretty box is a rendering.

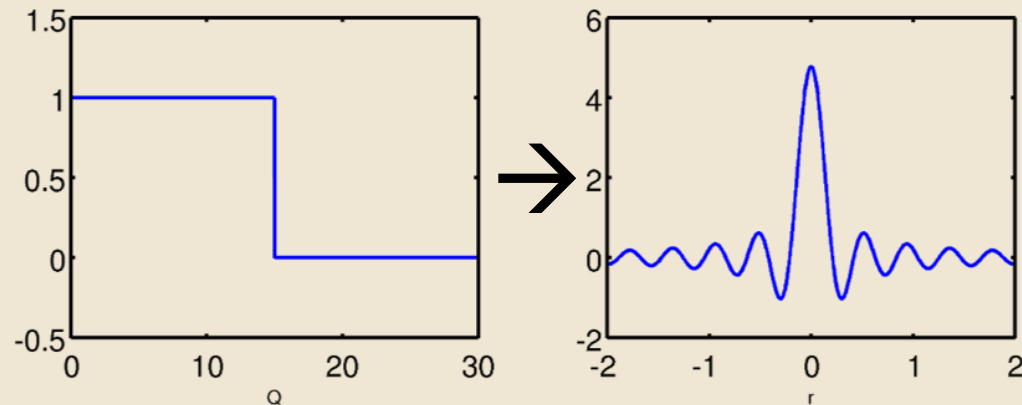
No average structure

If you cannot say what Bragg already told you, you are not ready for a local story.

How to publish a peak that does not exist

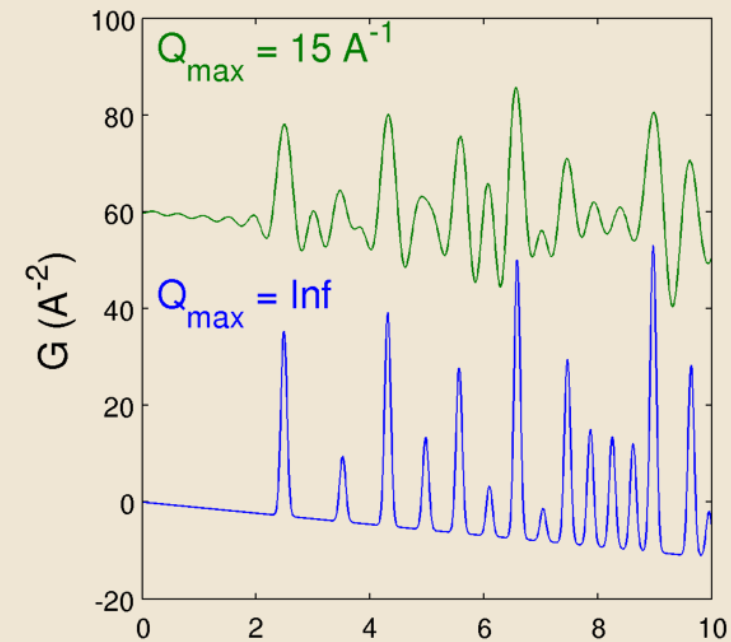
Effects from finite Q-range

$$G(r) = \frac{2}{\pi} \int_0^{Q_{\max}} F(Q) \sin Qr \, dQ$$

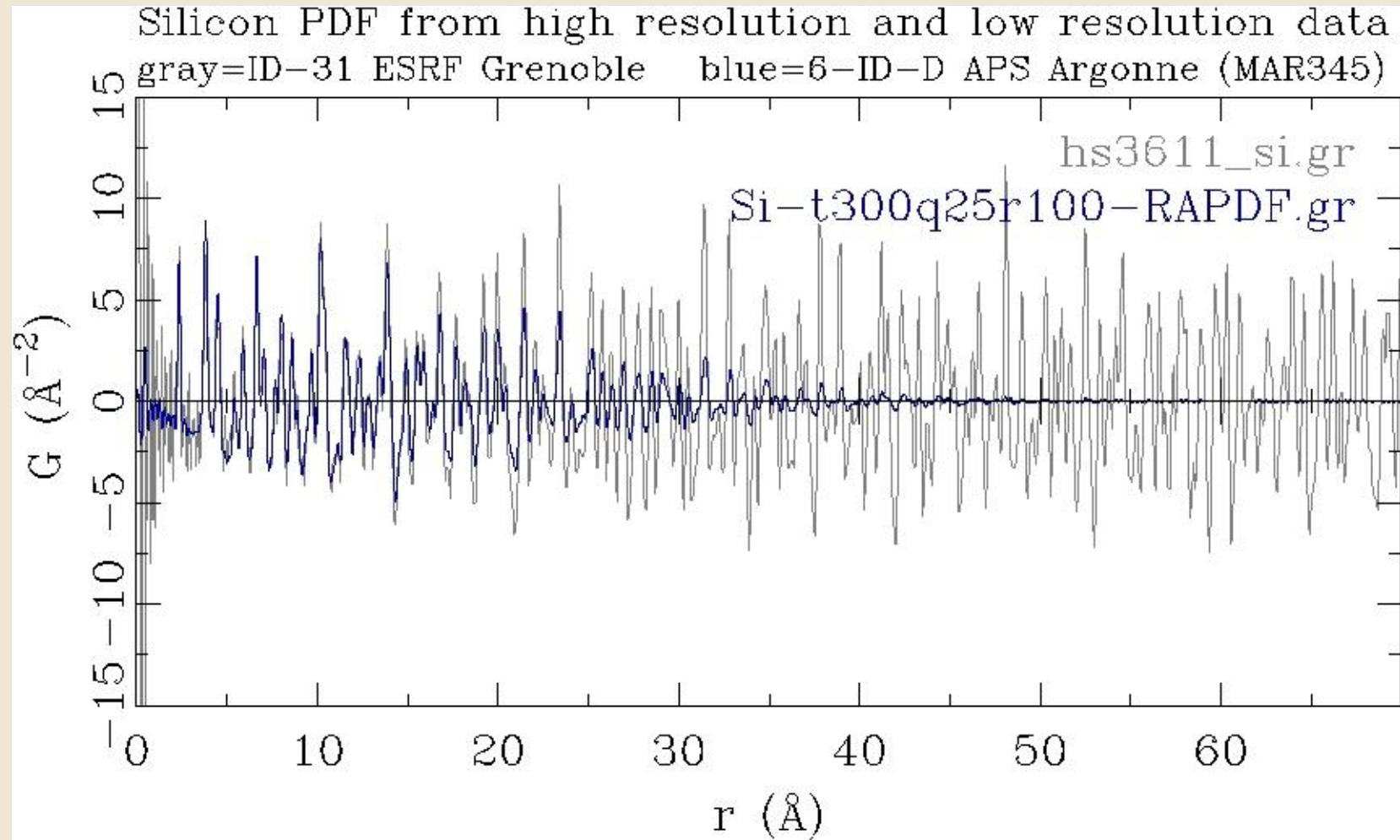


- ideal $F(Q)$ is multiplied by a step function
- $G(r)$ gets convoluted with a sinc function $\text{sinc}(r) = \sin(Q_{\max} r) / r \rightarrow r\text{-resolution} \approx \pi/Q_{\max}$
- **good r -resolution of G requires large $Q_{\max}$**
 $Q = 4\pi \sin \theta / \lambda \rightarrow$ best results with neutrons or high-energy x-rays

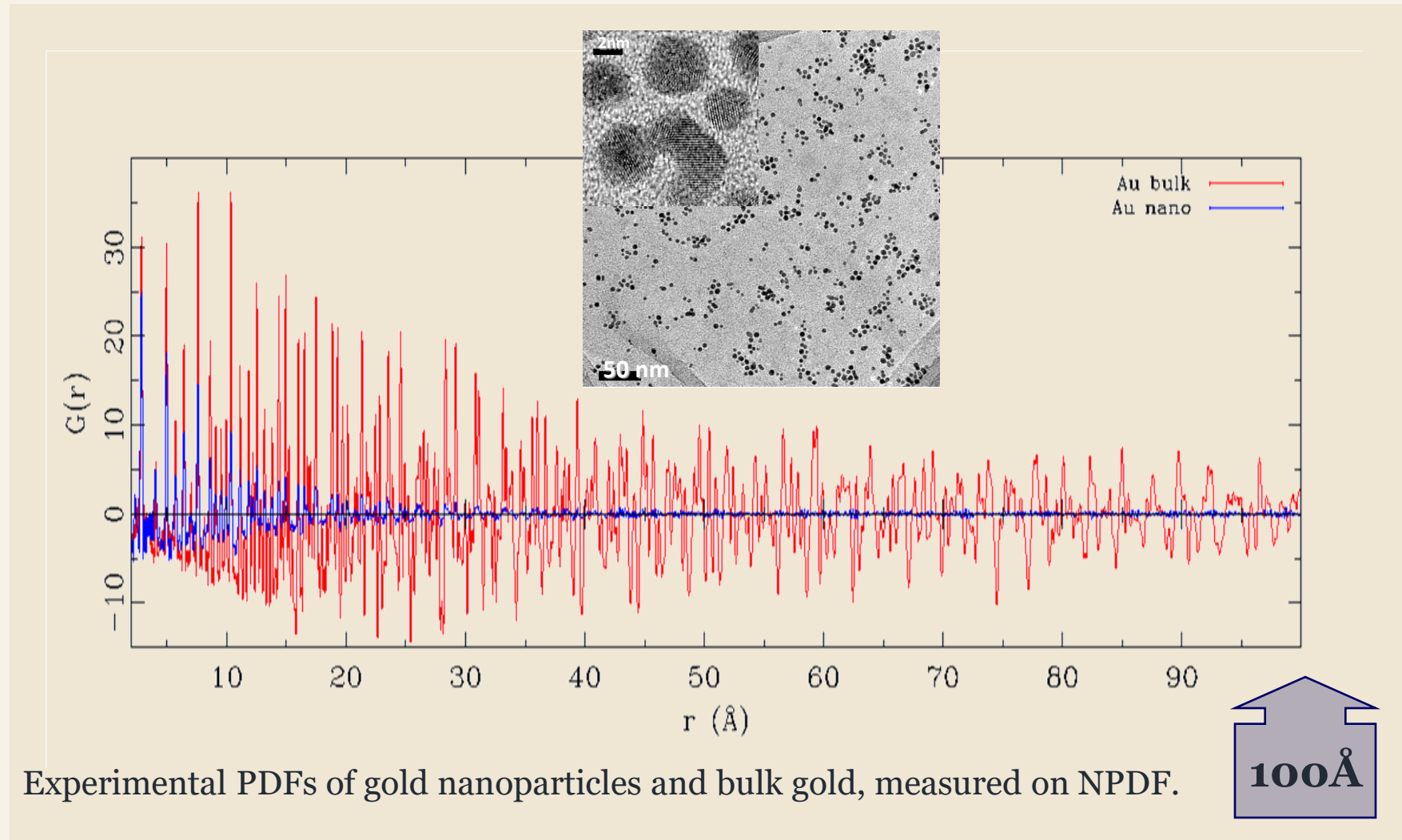
simulated nickel PDF



PDF: effect of the Q-space resolution



PDF: effect of the finite particle size – nano vs bulk



05

Case studies with references you can open tonight

Real materials, real puzzles, and real papers—with references you can open tonight and questions that will keep you up.

CdSe quantum dots: size, strain, stacking faults

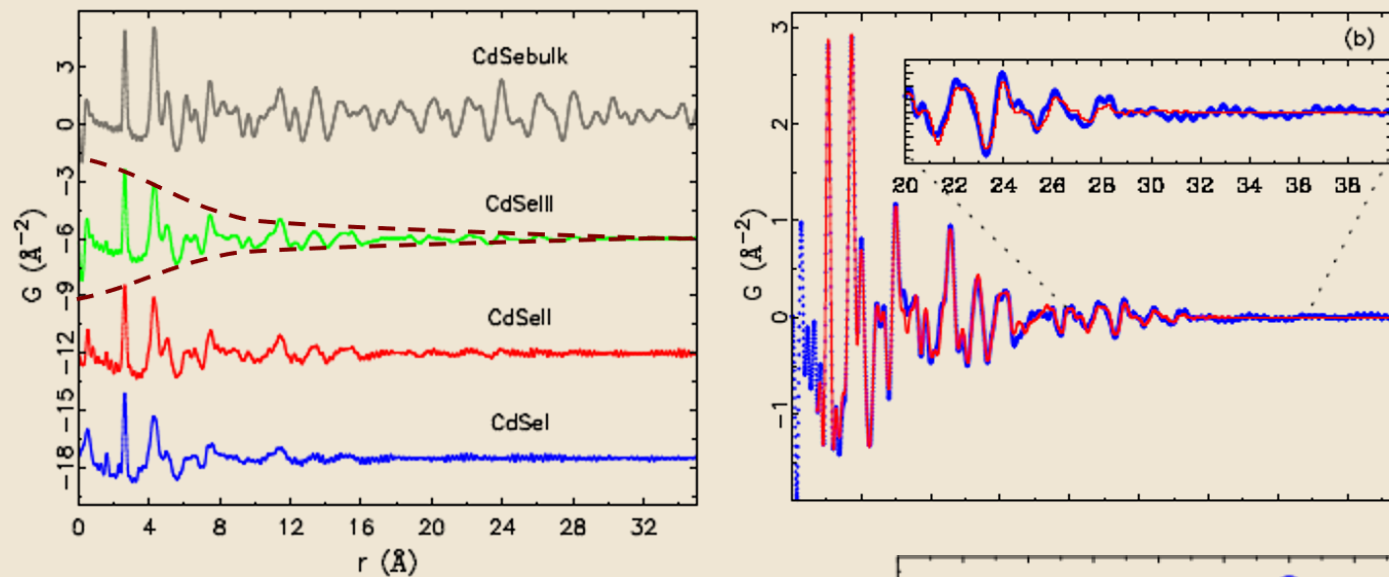
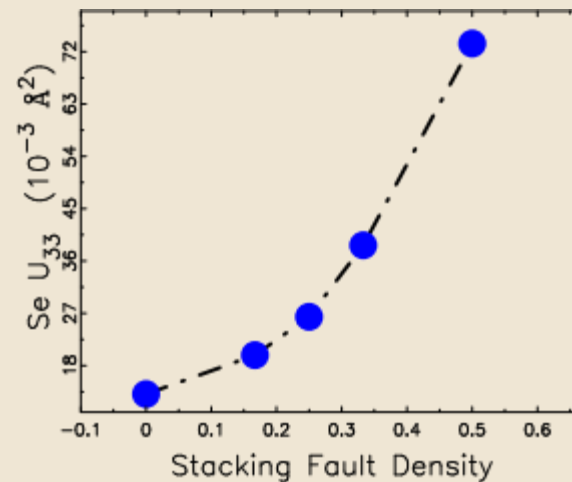
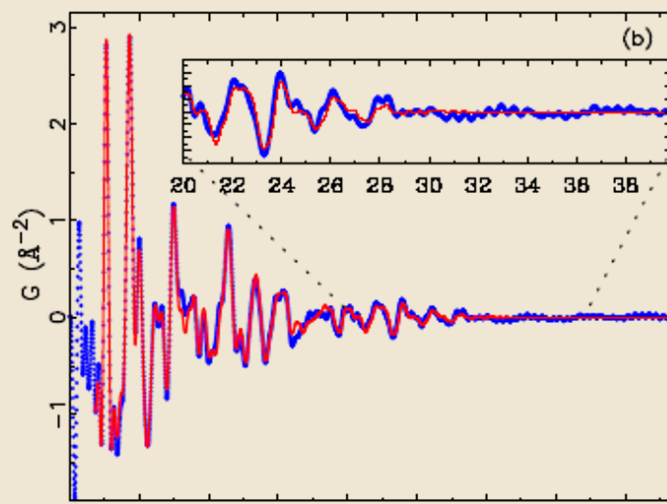


TABLE I: CdSe nanoparticle diameter as determined using various methods.

	CdSeIII	CdSeII	CdSeI
Nucleation time (s)	1200	630	15
Diameter (nm)			
TEM	3.5(2)	2.7(2)	2.0(2)
UV-vis	3.5(4)	2.9(3)	≤ 1.90
PL	3.6(4)	2.9(3)	≤ 2.1
PDF	3.7(1)	3.1(1)	2.2(2)



What PDF settled

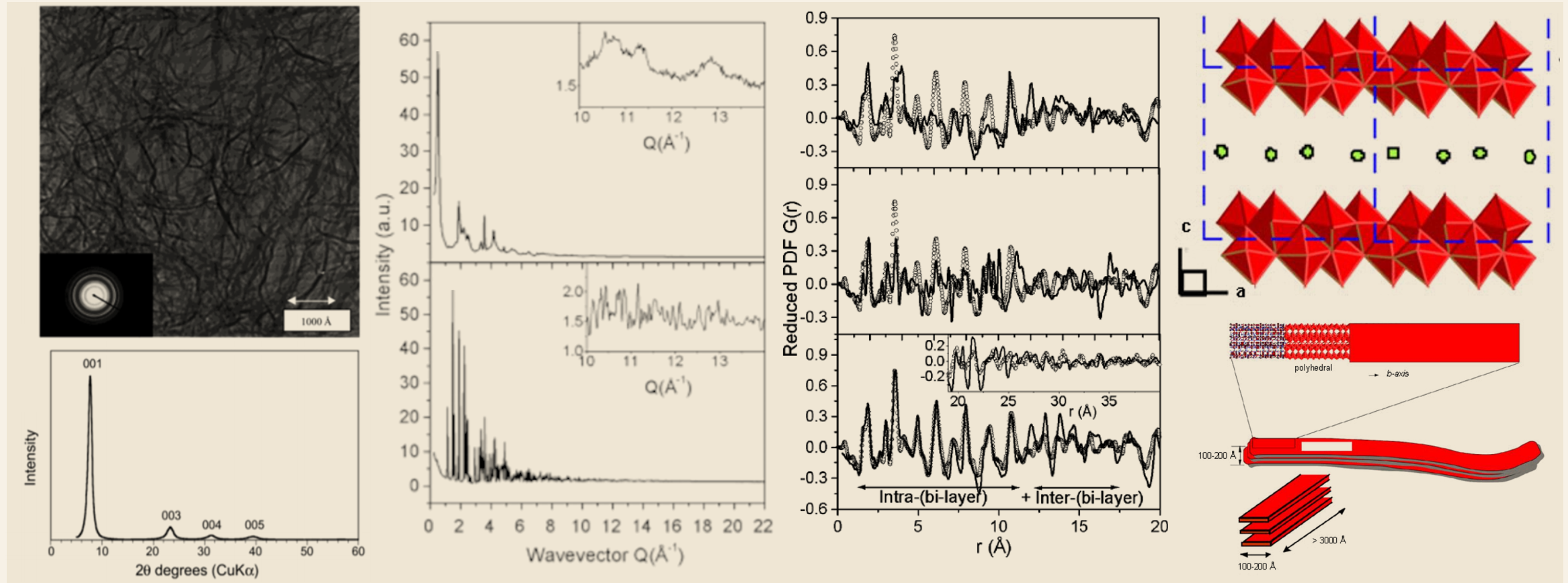
2–4 nm CdSe cores are wurtzite with ~50% stacking faults — not a novel crystal structure. Diameter from the $G(r)$ envelope matches TEM. Bond-length strain is measurable as a function of size.

Source

High-energy synchrotron X-ray PDF. Lab XRD cannot resolve the faulted stacking against the size envelope at this diameter.

A structure solution that Bragg could not start: $V_2O_5 \cdot nH_2O$ xerogel

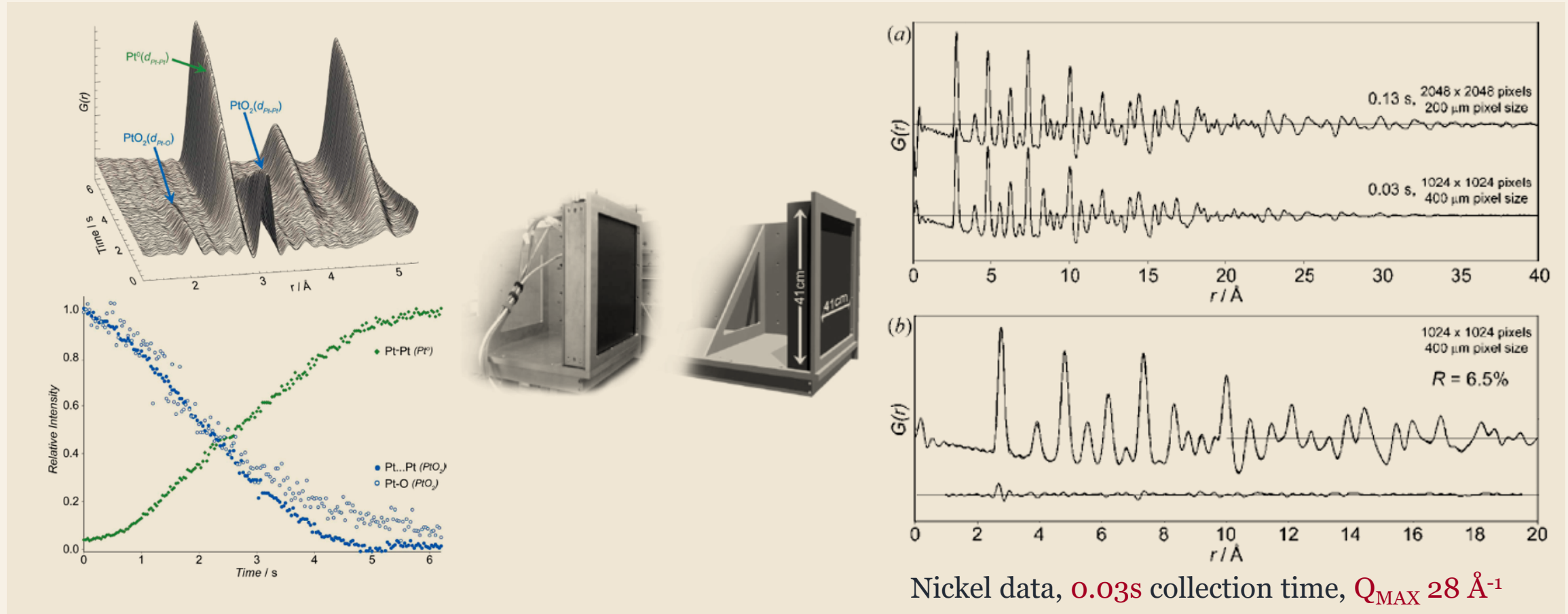
The xerogel is a battery and catalysis workhorse with almost no usable Bragg pattern. PDF showed the slabs are bilayers of square-pyramidal VO_5 , nearly crystalline locally, stacked with water in between.



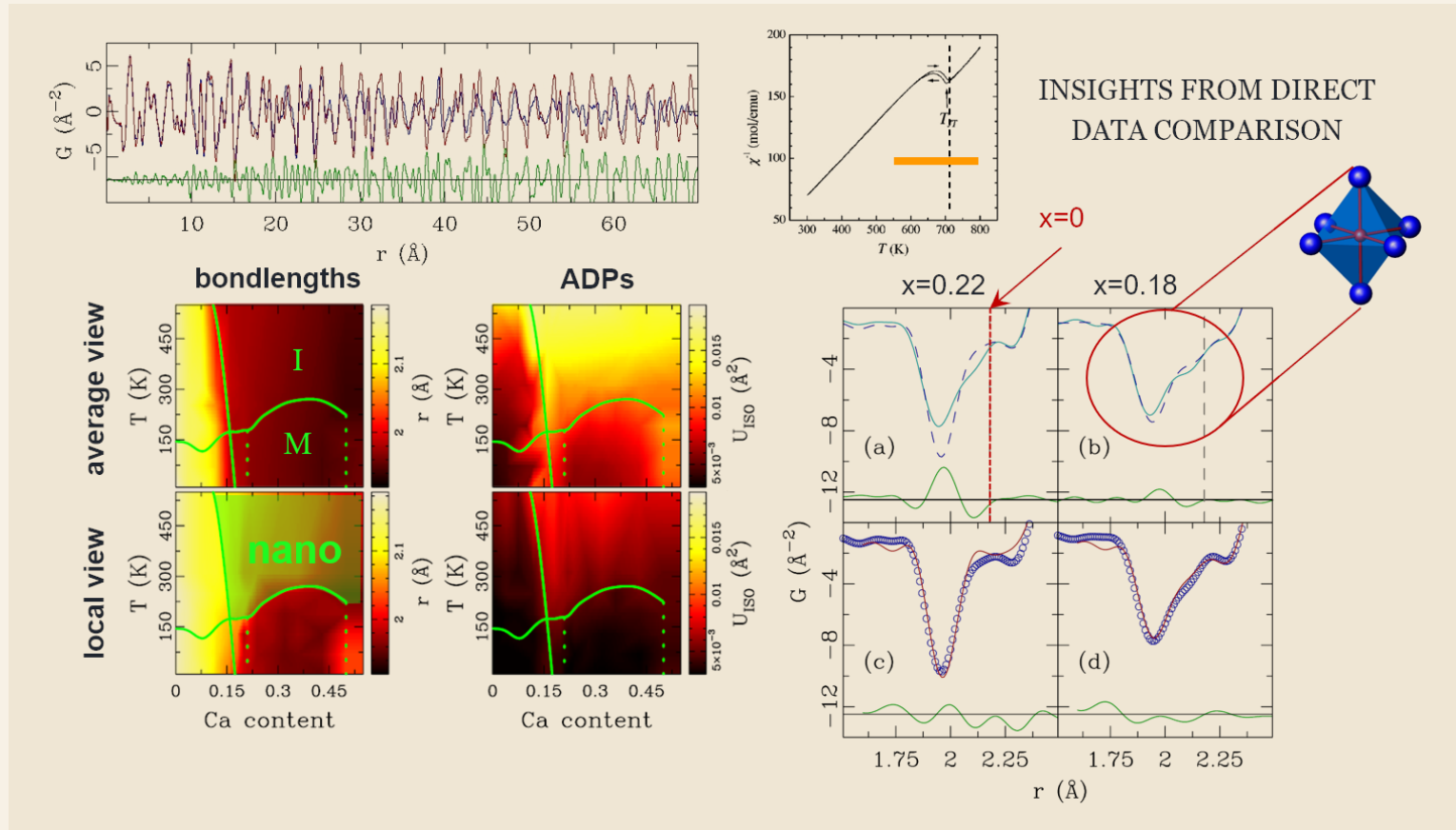
Petkov, Trikalitis, Božin, Billinge, Vogt & Kanatzidis, *J. Am. Chem. Soc.* 124, 10157 (2002). $V_2O_5 \cdot nH_2O$ xerogel.

Time-resolved PDF measurements: Reduction of $\text{Pt}^{\text{IV}} \rightarrow \text{Pt}^0$

Application of a large-area, high-sensitivity, fast readout, flat-panel GE detector based on an amorphous silicon



Manganites: the Jahn–Teller distortion that would not go away



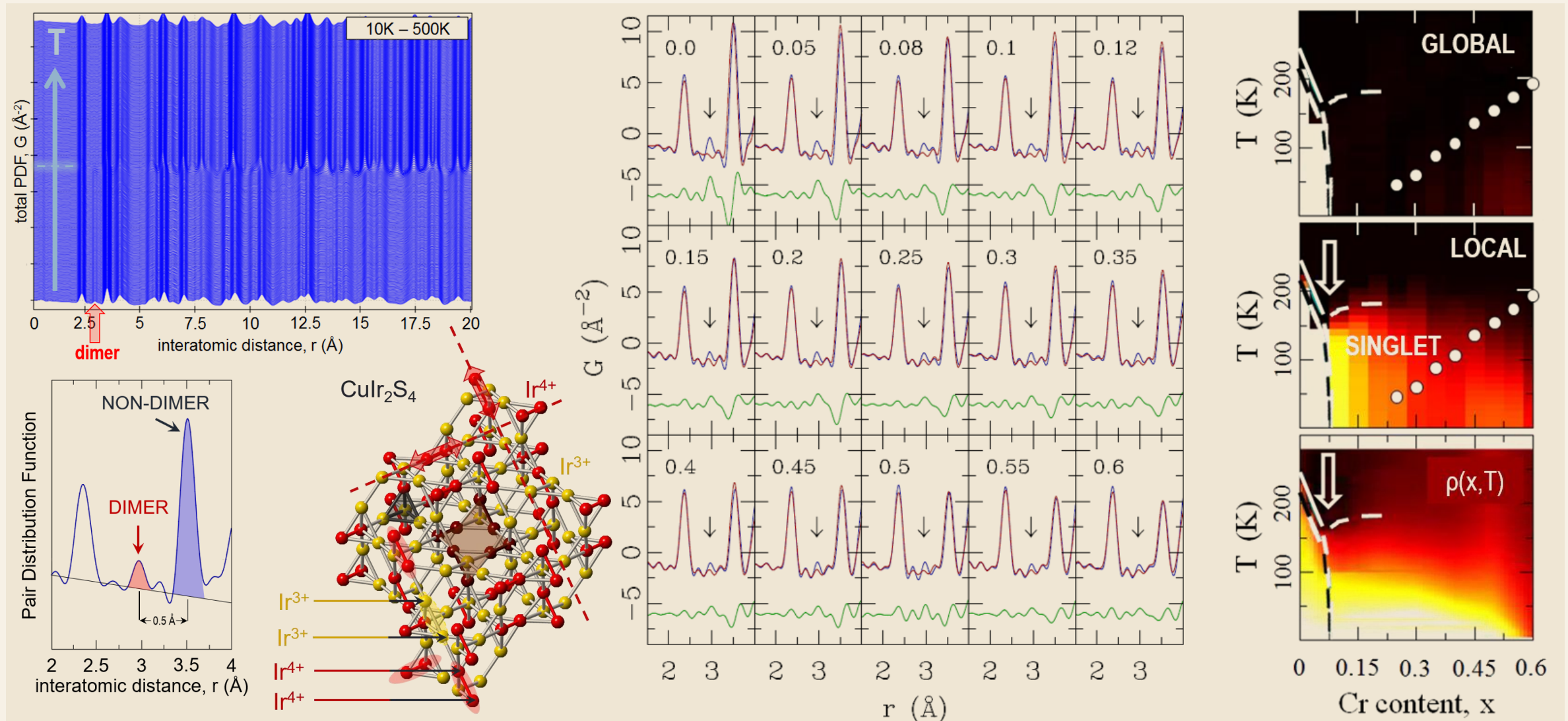
The claim

A local JT long-bond exists across the insulating side of the phase diagram. Its length is not constant — it shortens with Ca doping — contrary to a two-level small-polaron cartoon.

Why PDF

The average cell becomes metrically cubic. The first Mn–O shell in $G(r)$ does not.

Spin-singlet (dimer) formation w/o LRO: Cr-doped CuIr_2S_4 spinel



E. S. Bozin et al., *Sci. Rep.* 4, 4081 (2014);

Glasses and 'X-ray amorphous' molecular materials

What $G(r)$ gives you

First- and second-shell packing, chemical short-range order, and a medium-range length from the damping. A fingerprint that XRD of a halo cannot.

Lab vs synchrotron

A well-counted lab Ag/Mo PDF of silica is already a respectable glass fingerprint (Schertenleib 2025). Subtle intramolecular changes in pharmaceuticals want synchrotron Q_{MAX} .

Neutrons

Organic glasses without deuteration are an incoherent-H fight. Deuterate, or stay with X-rays and accept that H is a ghost.

Do not over-model

An RMC box of a glass will always look like a glass. Partial PDFs, NMR, and EXAFS are the adult supervision.

Electrons want in: ePDF

A TEM collects a total scattering pattern from a few nanometres of material. Fourier-transform it and you have an ePDF — local structure from a grain you can also image.

Temptation

Site-specific PDF of a single nanoparticle or an interface.

Tax

Multiple scattering, inelastic background, poor Q_{MAX} , and a community still writing the corrections.

Status

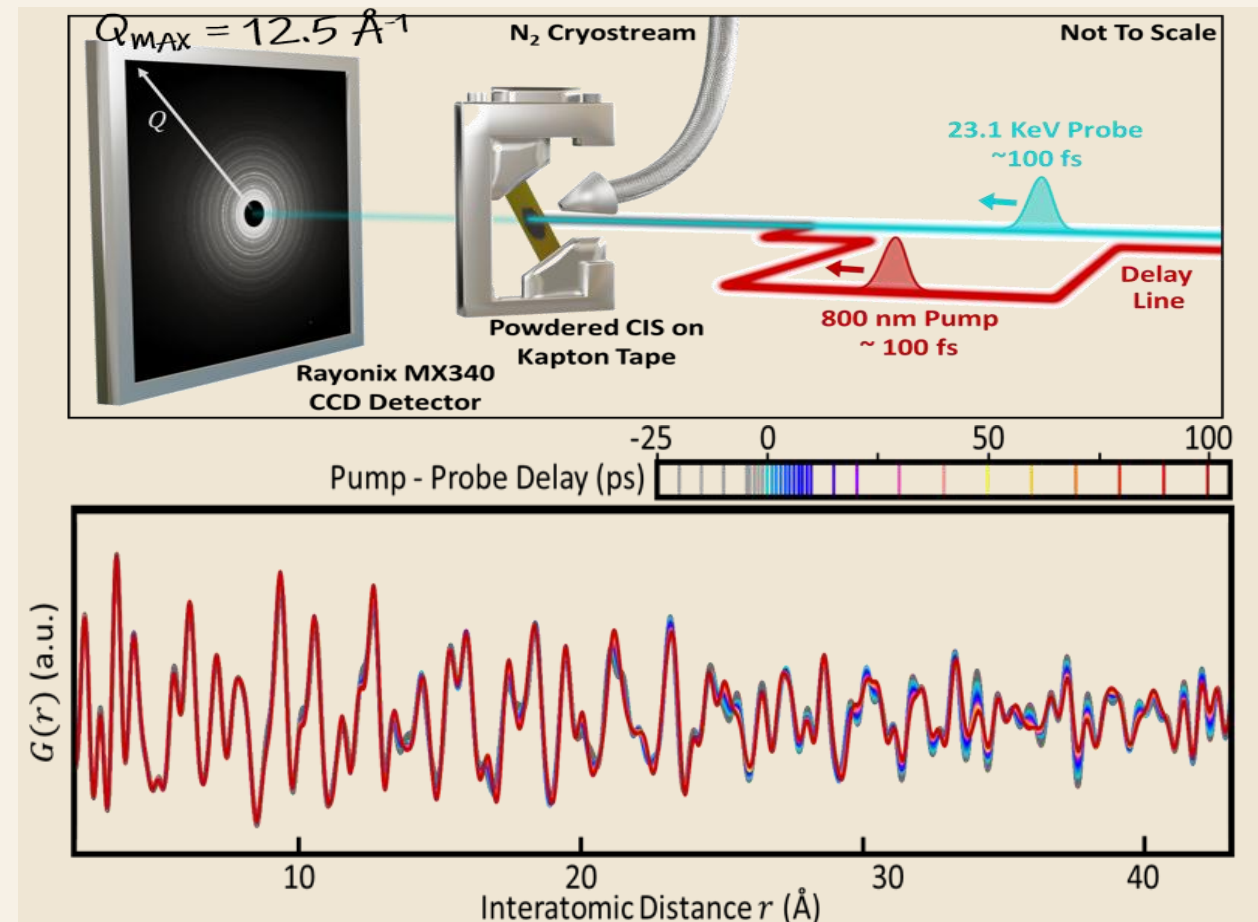
Works on selected nanocrystals when the background is treated as a scientific object, not a Photoshop layer.

Place in the toolkit

Complementary to synchrotron powder PDF, not a replacement. Same transform, **different systematic errors**.

Length-scale sensitive atomic “GPS”: uf-PDF

Ultrafast science captures matter in motion, revealing how structures evolve and transform in the fleeting moments when the world refuses to stand still. Proof of principle PDF at XFEL in pump-probe modality carried out – feasible but **very challenging**!



Griffiths, J., Suzana, A.F., Wu, L. et al. Resolving length-scale-dependent transient disorder through an ultrafast phase transition. *Nat. Mater.* 23, 1041–1047 (2024).

PDF is a team sport

Rietveld / SC-XRD

Long-range symmetry, weak superstructure, honest lattice.

EXAFS / XANES

Element-specific first shell; PDF gives all pairs and the medium range.

NMR / Mössbauer / EPR

Local chemistry; PDF is the geometric scaffold.

STEM / tomography

Rare defects, one grain; PDF averages 10^{18} cells without blinking.

Inelastic scattering

Dynamics vs static disorder. Peak widths are not ADPs.

DFT / MD / ML potentials

$G(r)$ is the experimental loss function those models should fear.

Software you can name on a slide without blushing

PDFgetX3 / PDFgetN

Ad-hoc X-ray reduction that made lab and RAPDF routine. **Pavol Juhás** et al., J. Appl. Cryst. 46, 560 (2013).

GudrunX / GudrunN

The serious neutron (and X-ray) correction pipeline from ISIS.

PDFgui / DiffPy-CMI

Small-box workhorses. Farrow et al. 2007; Juhás et al. 2015.

TOPAS / GSAS-II

If your group already lives there, PDF refinements can too.

RMCPProfile / fullrmc / EPSR

Large-box. Bring constraints.

PDFitc

Cloud apps for mining, similarity, NMF on operando series.

Where the photons and neutrons actually are

Class	Instruments (non-exhaustive)
Lab XRD PDF	Mo or Ag tube + area detector or point detector to 140° 2θ. Bruker D8 / Rigaku / Stoe variants now sold as PDF-capable.
Synchrotron PDF	NSLS-II 28-ID-1/2, APS 11-ID-B, DESY P02.1, Diamond I15-1, ESRF ID15A/ID31, SPring-8 BL04B2/BL08W.
Spallation n PDF	SNS NOMAD, POWGEN; ISIS GEM, POLARIS, NIMROD, SANDALS; J-PARC NOVA; formerly LANSCE NPDF.
Reactor n	ILL D4 — still the classic liquid/glass workhorse, lower Qmax than spallation.
3D / single crystal	Synchrotron monochromatic mesh scans; lab X-ray total-scattering goniometers.

A reading list that is not ornamental

1. T. Egami & S. J. L. Billinge, *Underneath the Bragg Peaks*, 2nd ed., Elsevier (2012). The book.
2. S. J. L. Billinge & I. Levin, *Science* 316, 561 (2007). The nanoscale problem, in two pages.
3. S. J. L. Billinge & M. G. Kanatzidis, *Chem. Commun.* 749 (2004). Nanostructure manifesto.
4. P. Juhás et al., *J. Appl. Cryst.* 46, 560 (2013). PDFgetX3.
5. C. L. Farrow et al., *J. Phys.: Condens. Matter* 19, 335219 (2007). PDFgui.
6. D. A. Keen, reviews of neutron total scattering (2022 and earlier). Source comparison tables.
7. T. Schertenleib et al., *Chem. Methods* (2025); arXiv:2406.18177. Lab PDF, done properly.
8. D. Hou et al., *J. Eur. Ceram. Soc.* 38, 971 (2018). Perovskite PDF review.
9. M. Terban & S. J. L. Billinge, *Chem. Rev.* 122, 1208 (2022). Molecular materials.
10. S. J. L. Billinge & K. M. Ø. Jensen, *Atomic Pair Distribution Function Analysis*, OUP (2023/24). Worked examples.

What to leave the hall believing (a.k.a. the summary)

- 1 Crystallography is the periodic average. Function often lives in the deviations.
- 2 $G(r)$ is total scattering, sine-transformed. Every pair, weighted, versus distance.
- 3 Lab Mo/Ag PDF is a real experiment if you count the high-Q tail and correct absorption.
- 4 Synchrotrons buy time, Q_{MAX} , and operando. Neutrons buy contrast and a flat form factor.
- 5 Start with peaks and a small box. Escalate only when the residual has a name.
- 6 A PDF without Q_{MAX} , Q_{DAMP} and an average-structure sentence is a rumour.

Answers I would like to be asked

Is lab PDF 'good enough'?

For screening, teaching, coarse local order, and amorphous fingerprints — yes, if you follow Schertenleib-class protocols. For 0.1 Å bond splits and operando — no.

Why not always neutrons?

Sample mass, H, access, and the fact that many questions are heavy-atom questions.

Can PDF see magnetism?

mPDF from magnetic neutron scattering. Same sine transform, spin pairs instead of nuclear pairs.

How small a particle?

A well-defined first shell at 1 nm; a refined structure type often by 2–3 nm. Below that you are doing molecular PDF.