Recent and future developments in PDF-land

S.J.L. Billinge

CMPMS, Brookhaven National Laboratory

Department of Applied Physics and Applied Mathematics

Columbia University,

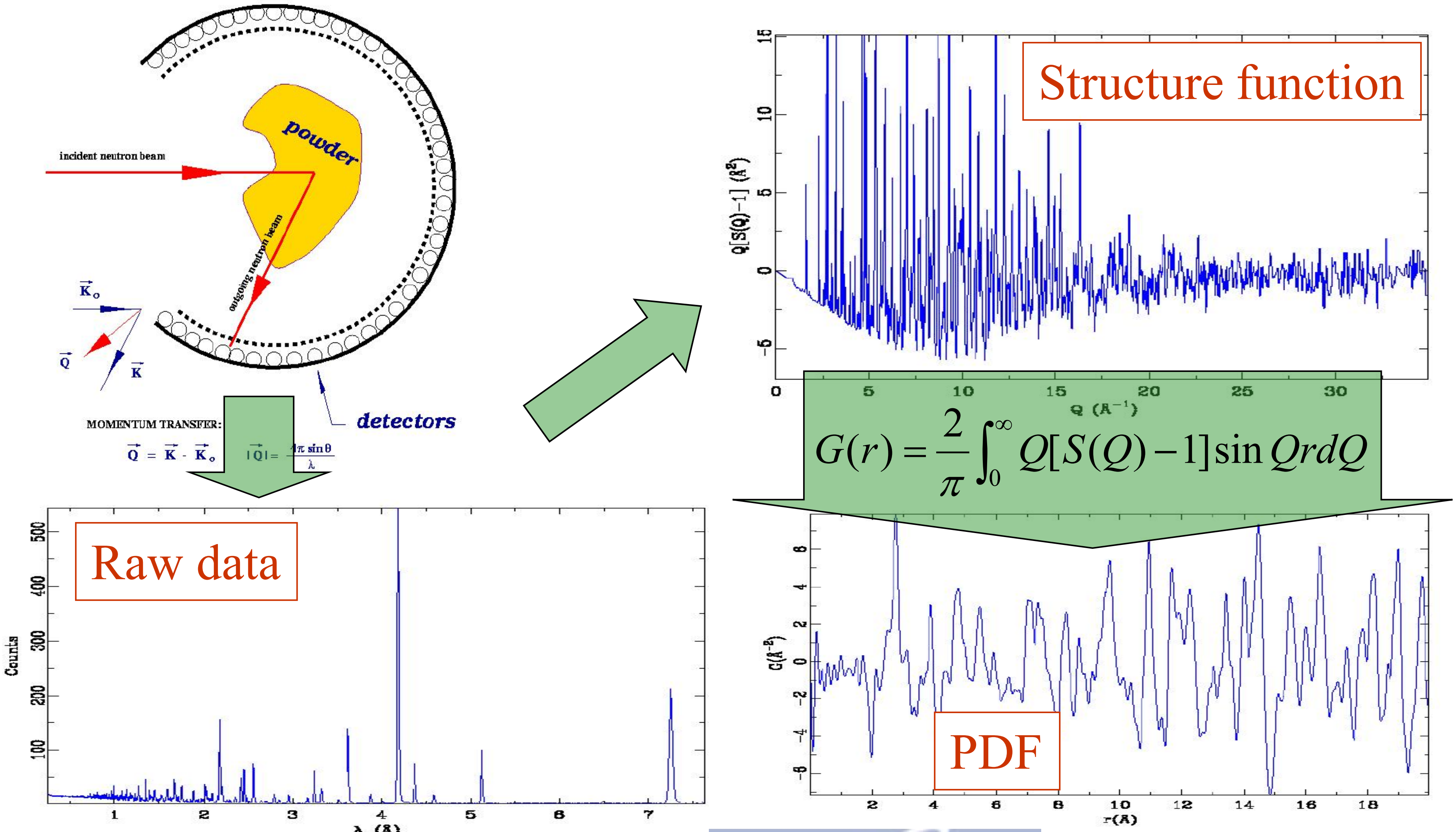
http://thebillingegroup.com

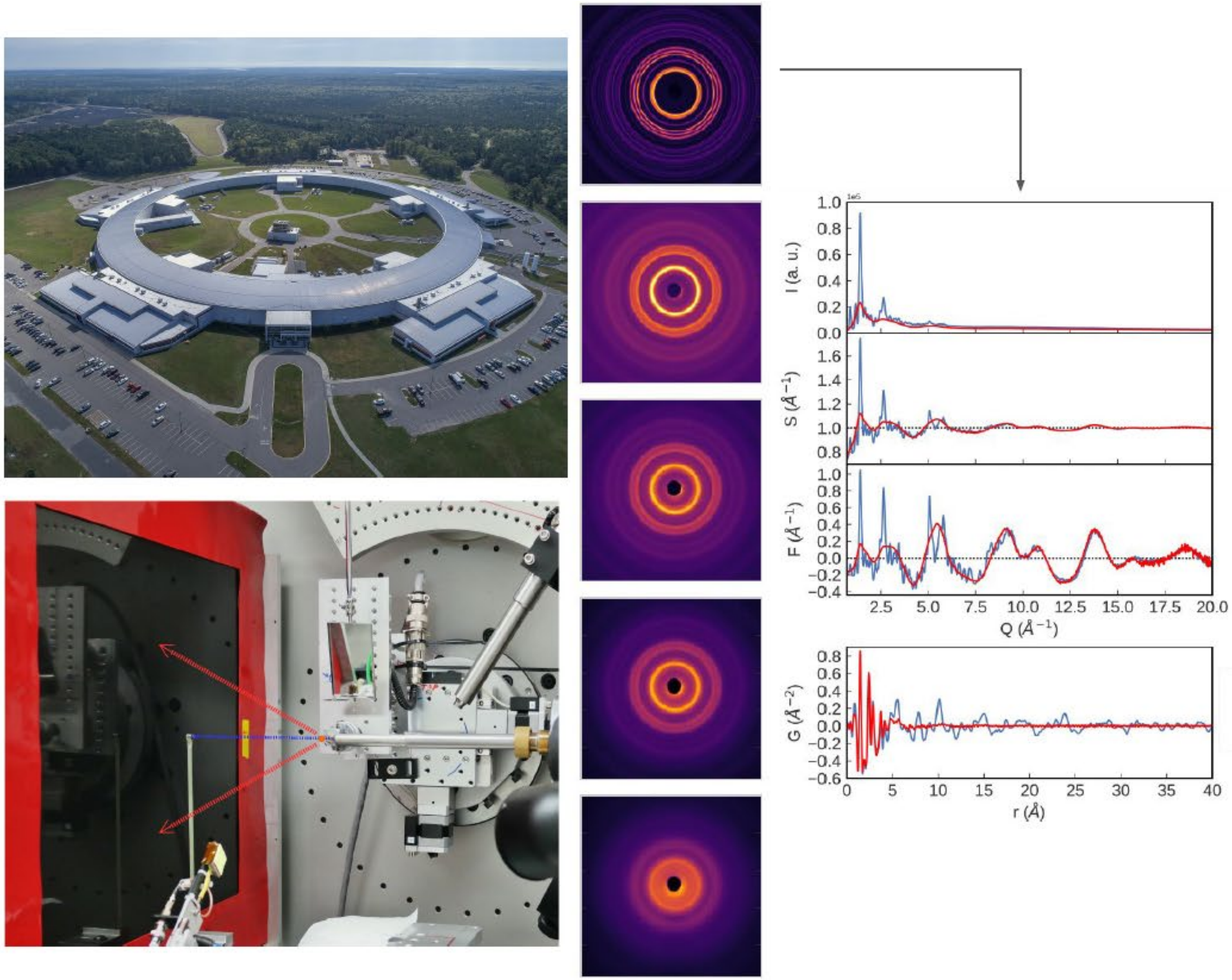
Overview

1. What is PDF (brief)?
2. Small sample of science that can be done with PDF
3. What is the state of the art in PDF methodology
    1. Time resolved studies
        1. In situ measurements
        2. Ultra-fast PDF
    2. Spatially resolved studies
        1. Scanning nanostructure X-ray microscopy
        2. Scanning nanostructure Electron microscopy
    3. Textured samples and samples with preferred orientation
    4. High throughput analysis and modeling
        1. Automasking of 2D images
        2. Feature tracking
        3. Non Negative Matrix Factorization
        4. High throughput modeling

What is PDF

The atomic Pair Distribution Function





$$S(Q)-1=\frac{I(Q)}{N\langle f\rangle^2}-\frac{\langle f^2\rangle}{\langle f\rangle^2}$$

Normalize by scattering cross section

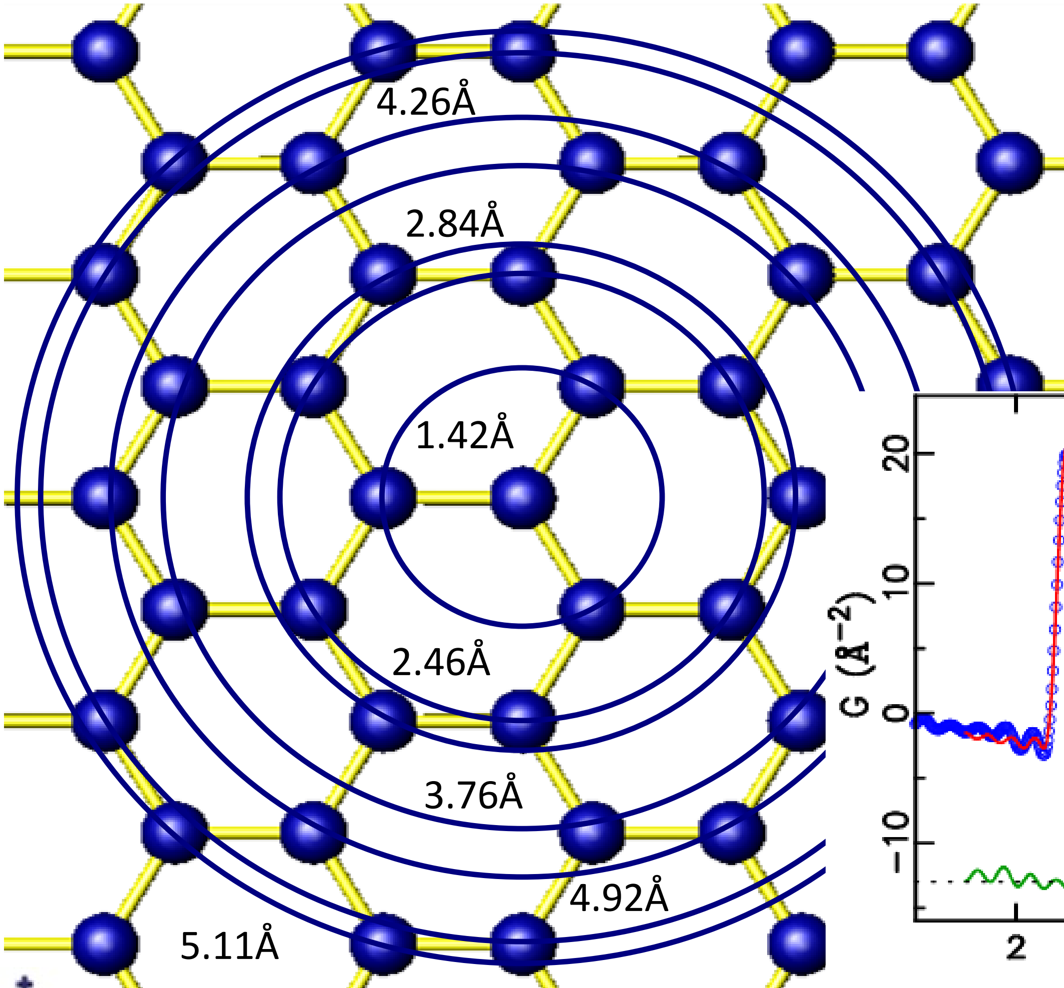
$$F(Q)=Q[S(Q)-1]$$

Transform to physical units

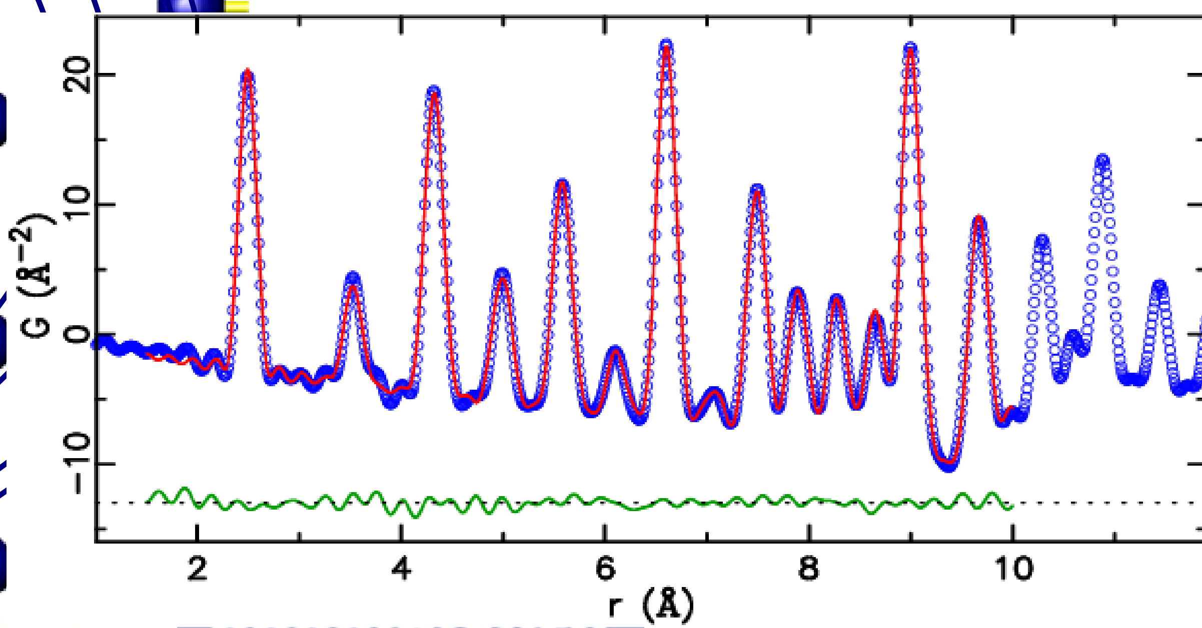
$$G(r)=\frac{2}{\pi}\int_{Q_{min}}^{Q_{max}} F(Q)\sin(Qr)\,dQ$$

Fourier transform

Nanostructure refinement



Pair distribution function (PDF) gives the probability of finding an atom at a distance “r” from a given atom.



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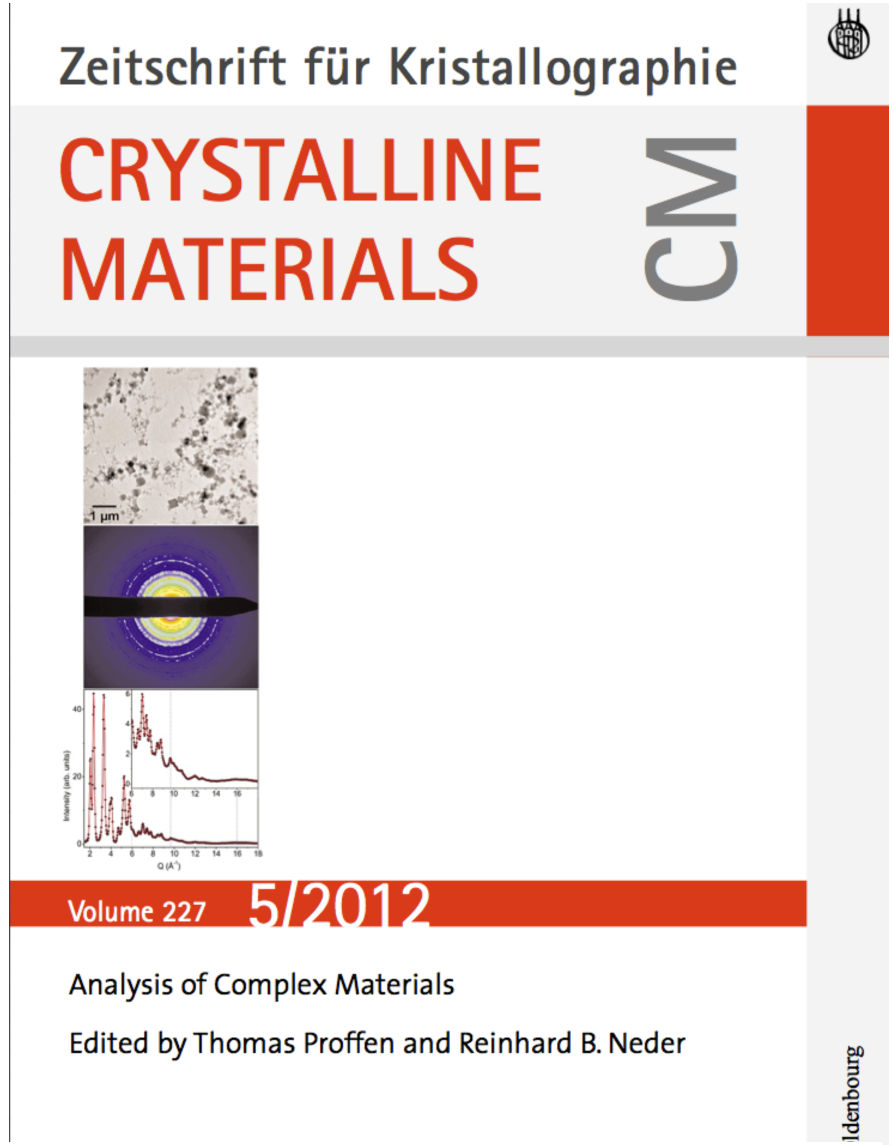
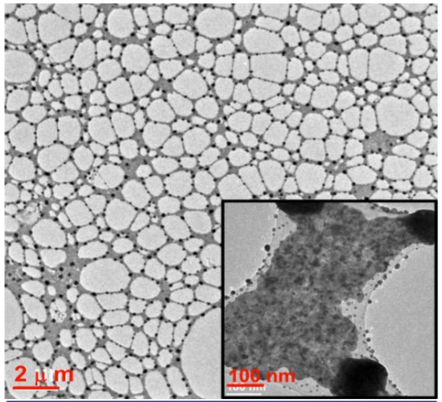
PDFs from laboratory microscopes

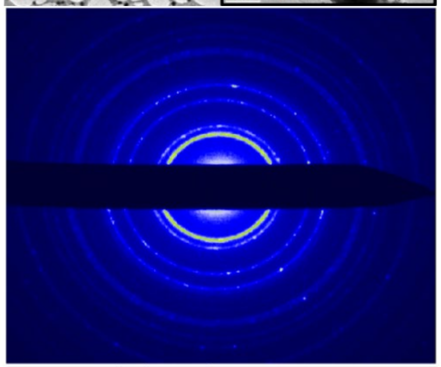


- Milinda Abeykoon, SJLB et al, *Z. Kristallogr.* **227**, 248-256 (2012)
- Abeykoon, SJLB, et al., *J. Appl. Crystallogr.* **48**, 244-251 (2015)

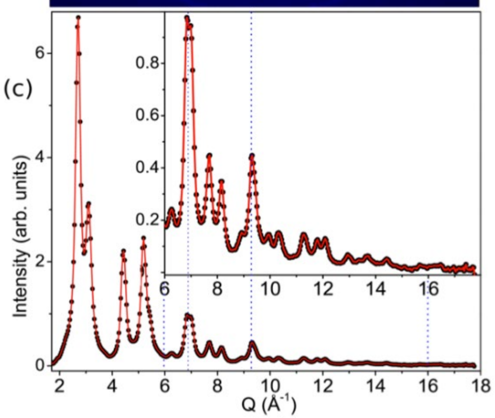
Au (1000) Å particles



(b)

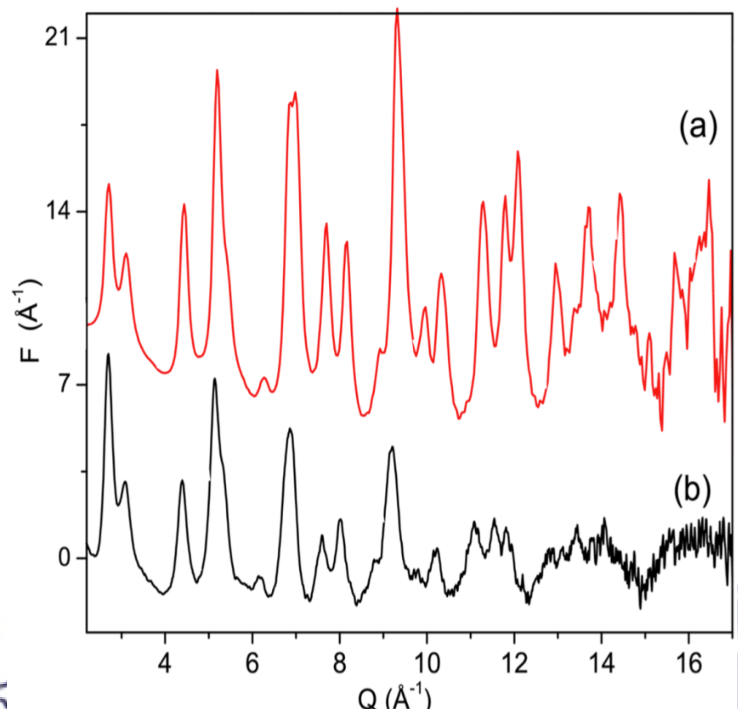


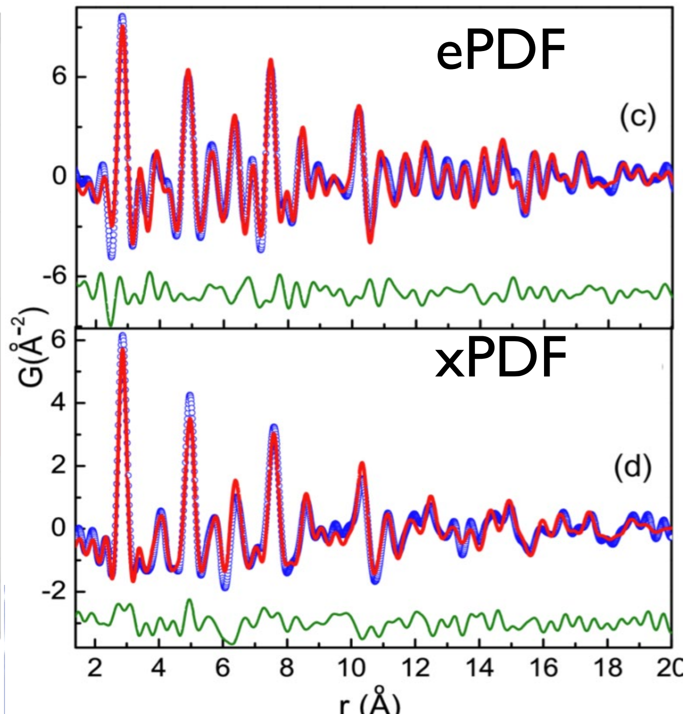
(c)



	ePDF (film)	ePDF (NP)	xPDF
$Q_{\max}$ ($Å^{-1}$)	15.25	15.25	15.25
Fit range (Å)	1–20	1–20	1–20
Cell parameter (Å)	4.075(3)	4.076(2)	4.058(1)
U_{iso} ($Å^2$)	0.033(4)	0.006 (3)	0.014(1)
Diameter (Å)	~27[a]	~1000[b]	24.51(9)
Q-damp ($Å^{-1}$)	0.095(5)	0.095(5)	0.047(2)
Rw (%)	17	24	20

a: film thickness measured during deposition
b: NP diameter estimated directly from the TEM image





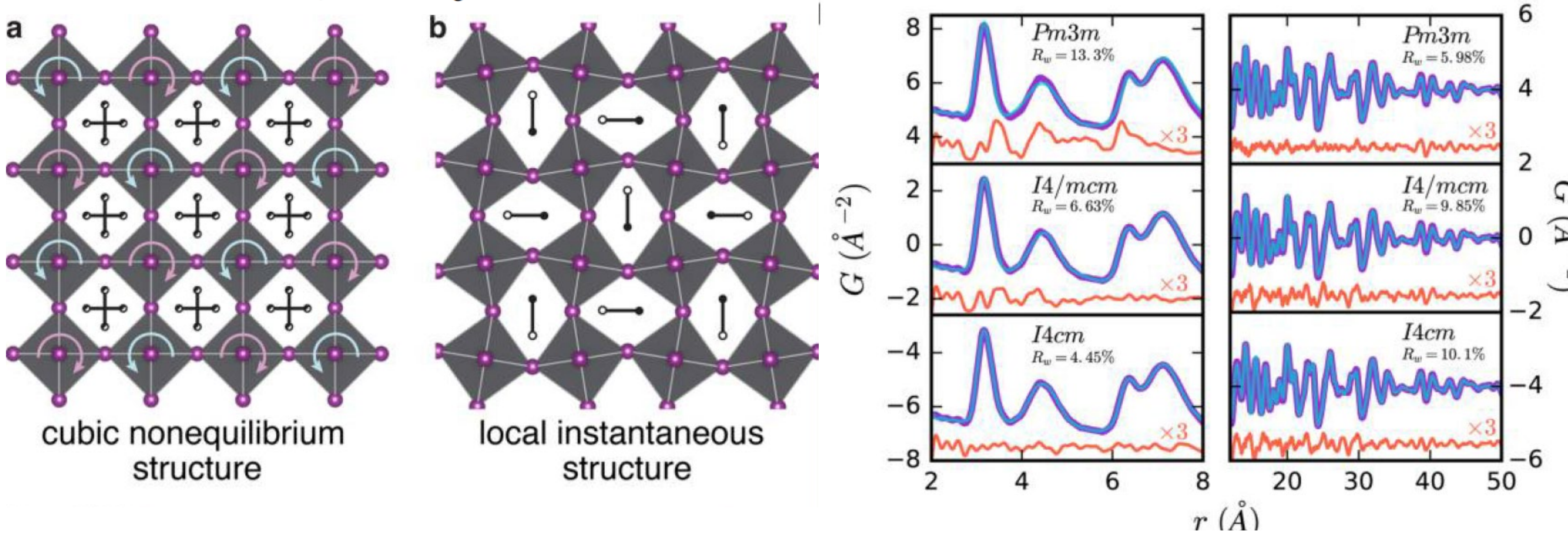
What science can be done with PDF?

ACS Energy Letters
ACS AuthorChoice
http://pubs.acs.org/journal/aelccp

LETTER

Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite

Alexander N. Beecher,[†,⊥] Octavi E. Semonin,[†,⊥] Jonathan M. Skelton,[‡] Jarvist M. Frost,[‡] Maxwell W. Terban,[¶] Haowei Zhai,[¶] Ahmet Alatas,[§] Jonathan S. Owen,[†] Aron Walsh,[‡] and Simon J. L. Billinge*,[¶,∥]



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PCCP

RSC Publishing

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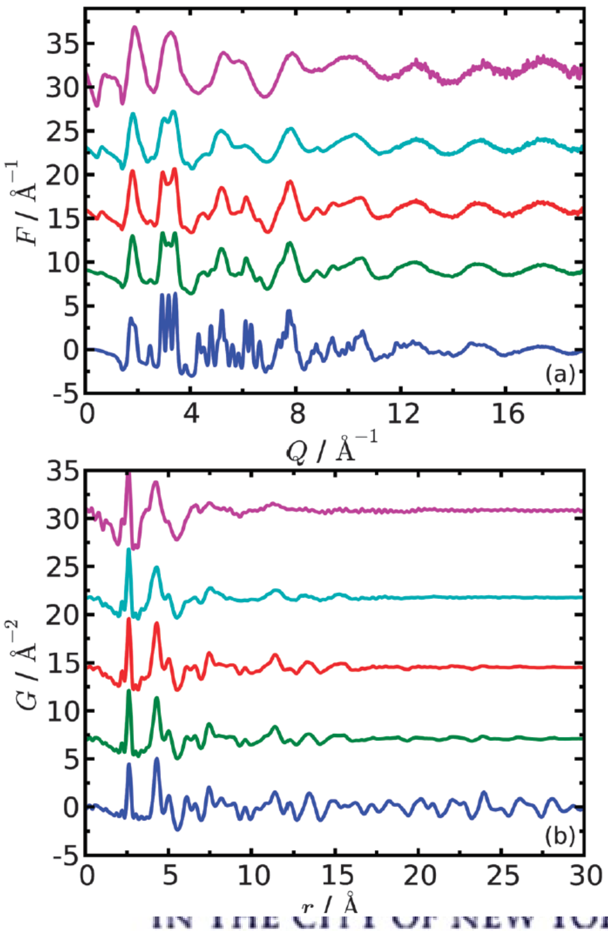
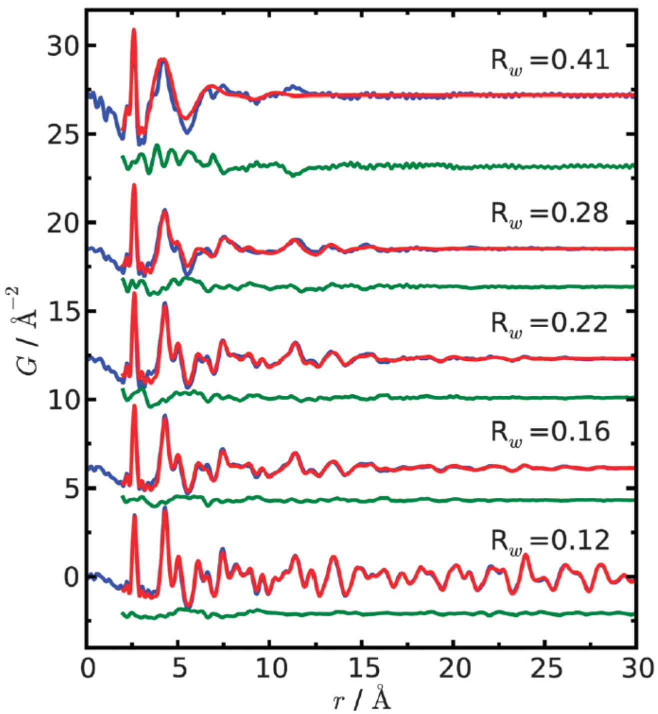
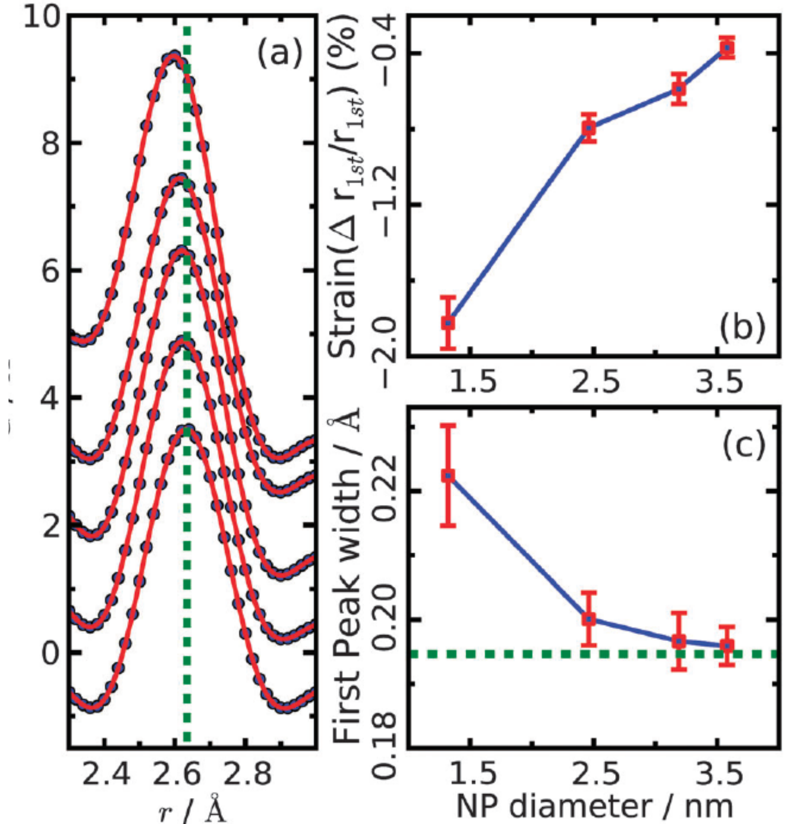
Cite this: *Phys. Chem. Chem. Phys.*, 2013, **15**, 8480

Confirmation of disordered structure of ultrasmall CdSe nanoparticles from X-ray atomic pair distribution function analysis

Xiaohao Yang,[a] Ahmad S. Masadeh,[b] James R. McBride,[c] Emil S. Božin,[d] Sandra J. Rosenthal[c] and Simon J. L. Billinge*[ad]







nature COMMUNICATIONS

ARTICLE

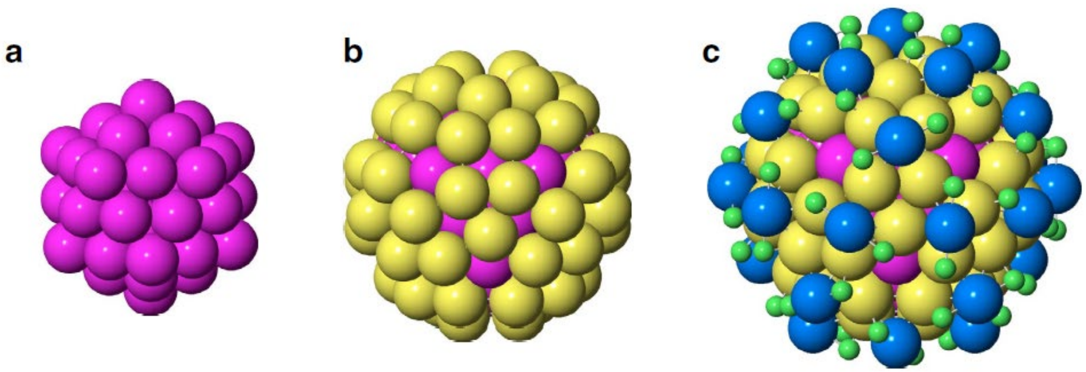
Received 22 Aug 2015 | Accepted 6 May 2016 | Published 14 Jun 2016

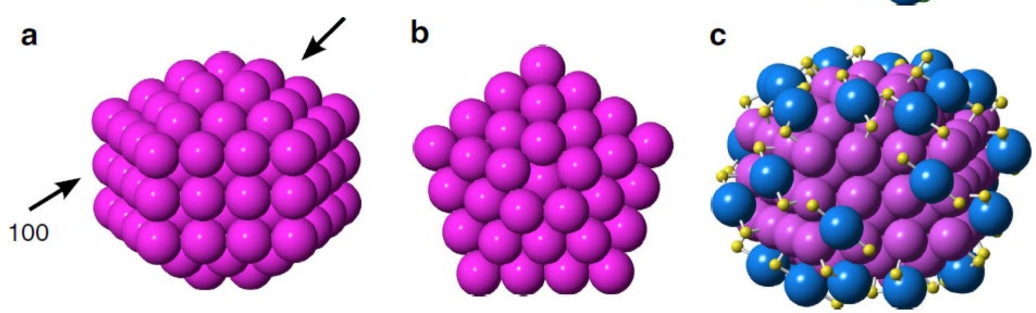
DOI: 10.1038/ncomms11859

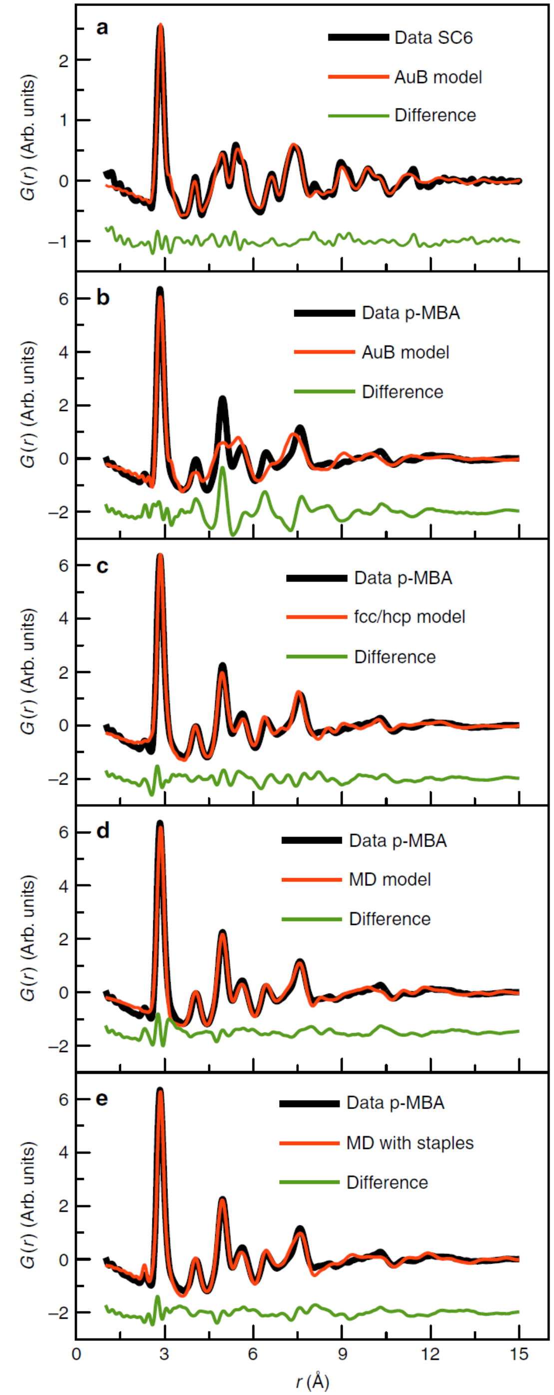
OPEN

Polymorphism in magic-sized $Au_{144}(SR)_{60}$ clusters

Kirsten M.Ø. Jensen[1,*], Pavol Juhas[2,*], Marcus A. Tofanelli[3], Christine L. Heinecke[3], Gavin Vaughan[4], Christopher J. Ackerson[3] & Simon J.L. Billinge[1,2]



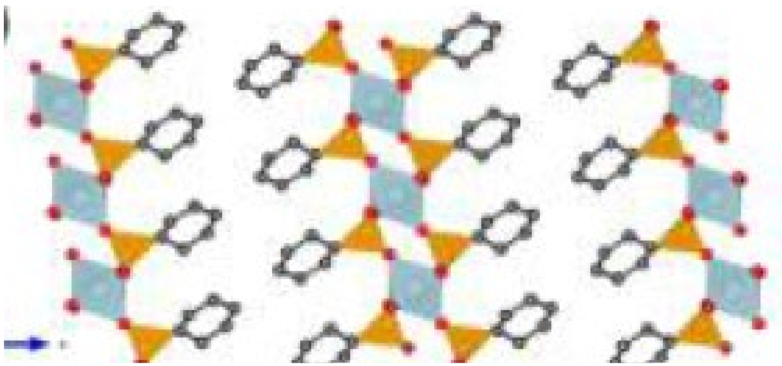


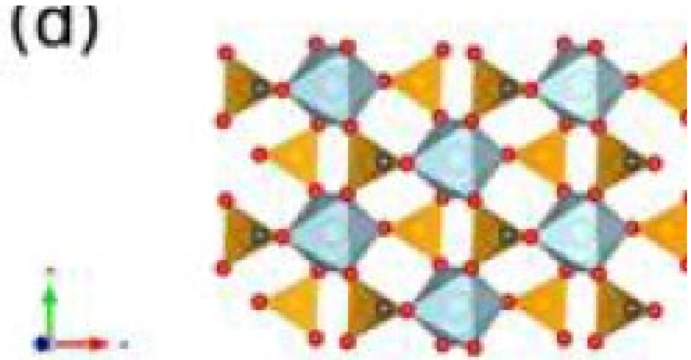


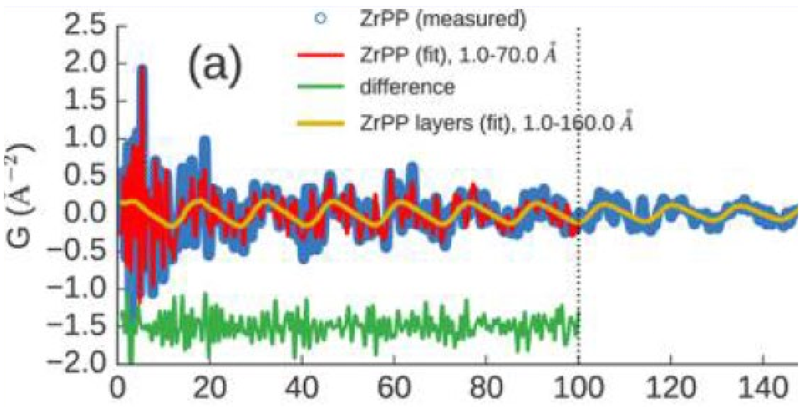
Inorganic Chemistry
Article
pubs.acs.org/IC

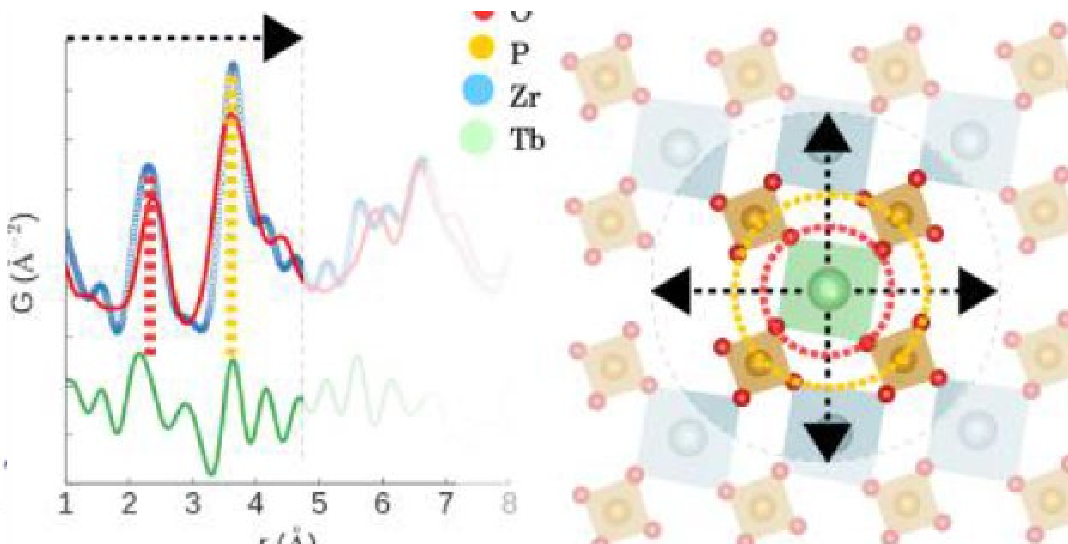
Local Environment of Terbium(III) Ions in Layered Nanocrystalline Zirconium(IV) Phosphonate–Phosphate Ion Exchange Materials

Maxwell W. Terban,[#,†] Chenyang Shi,[#,†] Rita Silbernagel,[‡] Abraham Clearfield,[‡] and Simon J. L. Billinge[*,†,⊥]









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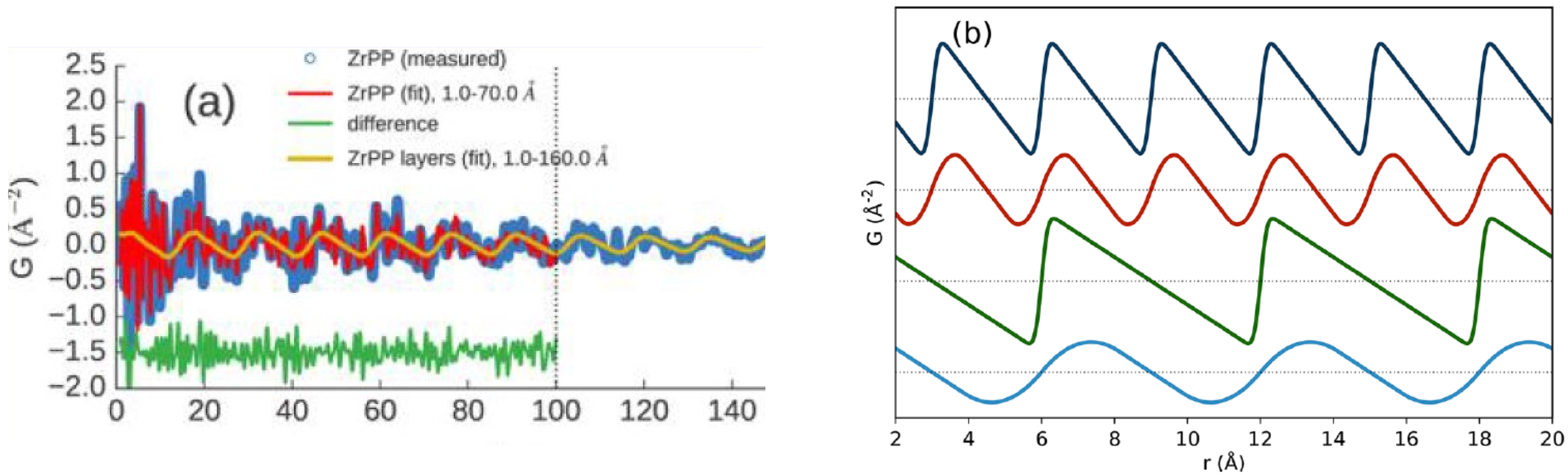
CHEMICAL REVIEWS

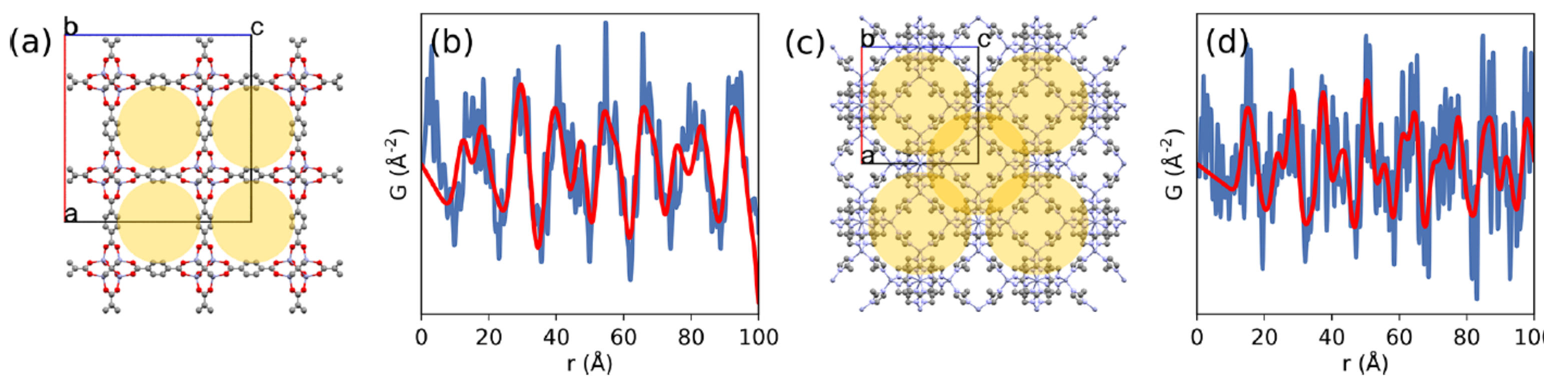
pubs.acs.org/CR

Review

Structural Analysis of Molecular Materials Using the Pair Distribution Function

Maxwell W. Terban* and Simon J. L. Billinge*





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Nanoscale

PAPER

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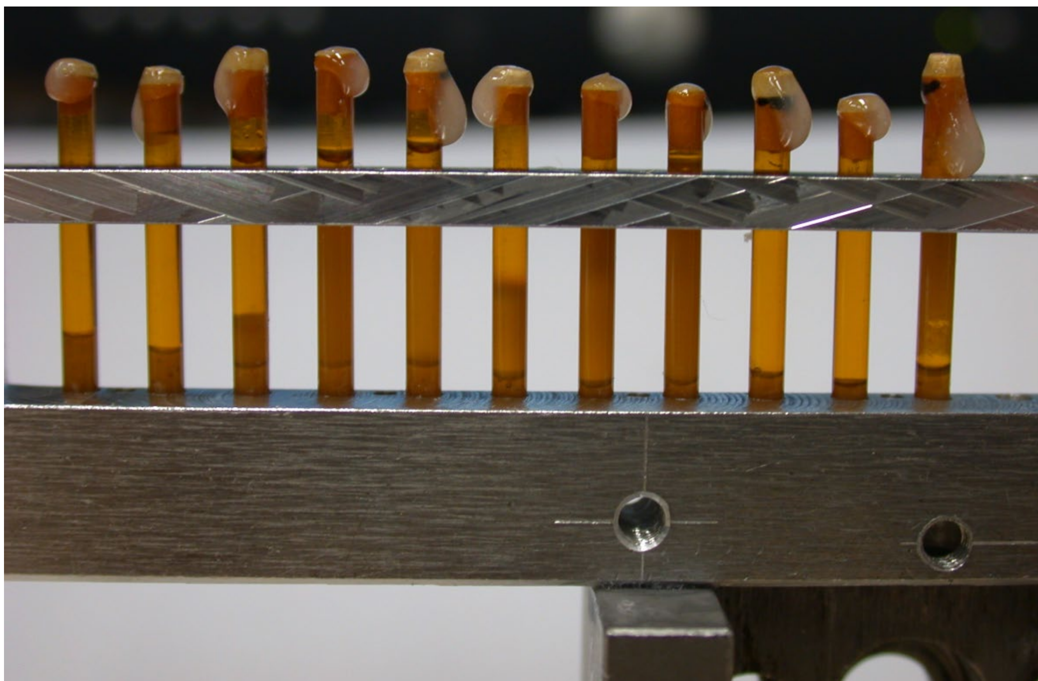
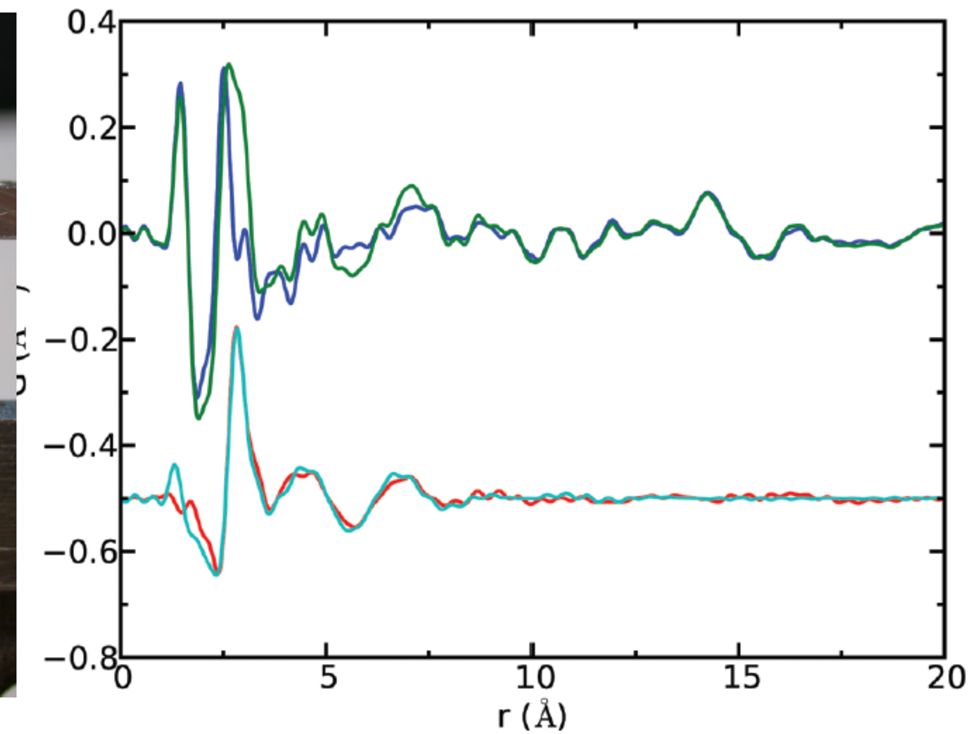
Cite this: *Nanoscale*, 2015, **7**, 5480

Detection and characterization of nanoparticles in suspension at low concentrations using the X-ray total scattering pair distribution function technique

Maxwell W. Terban,[a] Matthew Johnson,†[b] Marco Di Michiel[c] and Simon J. L. Billinge*[a,d]





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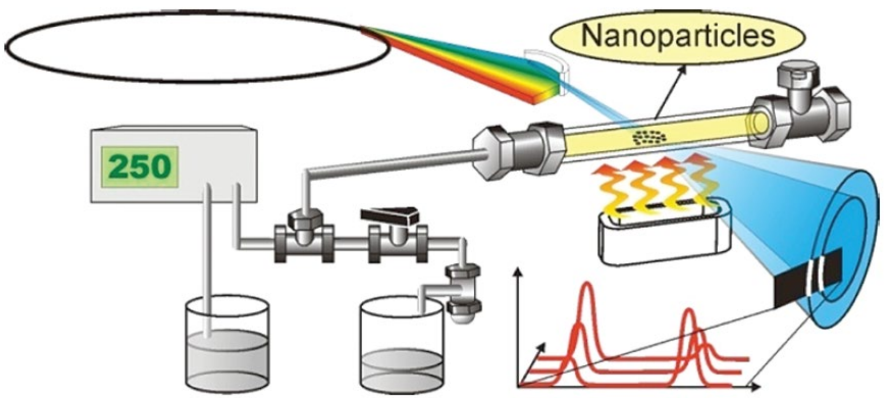
Time resolved PDF

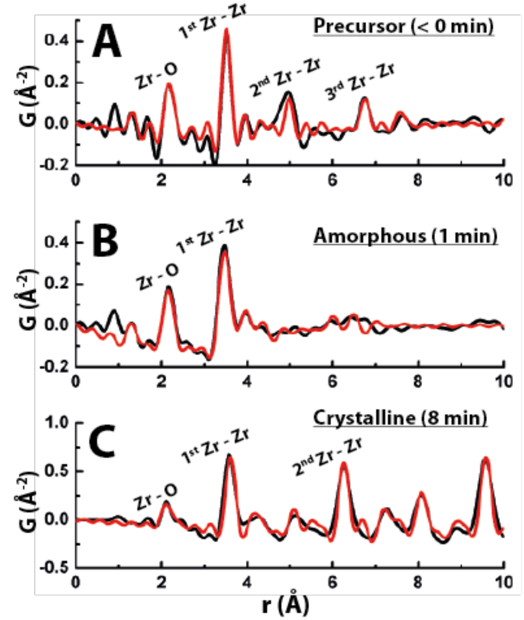
In situ studies

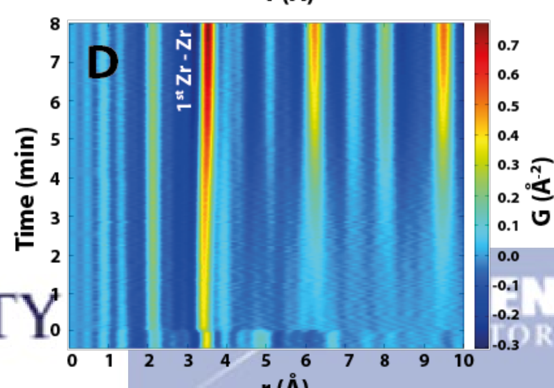
IUCrJ
ISSN 2052-2525
CHEMISTRY | CRYSTENG

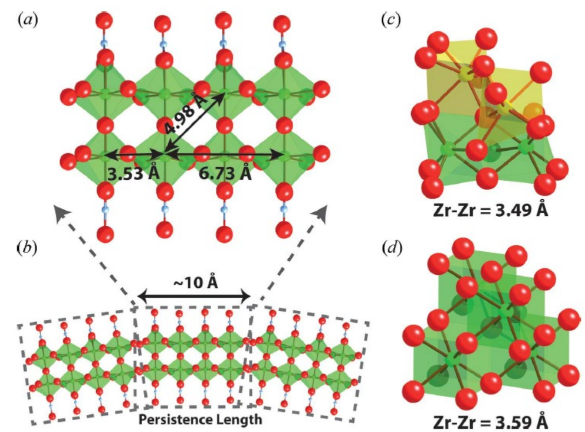
Evolution of atomic structure during nanoparticle formation

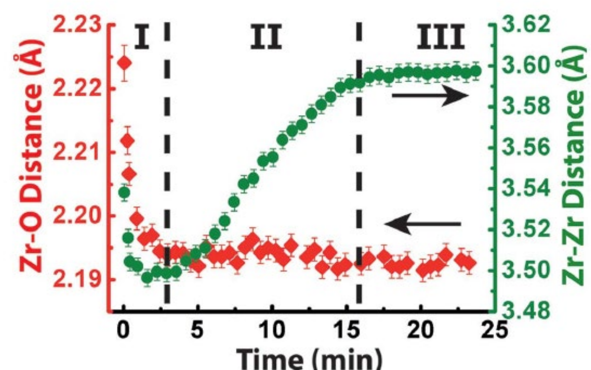
Christoffer Tyrsted,[a] Nina Lock,[a,b] Kirsten M. Ø. Jensen,[a,c] Mogens Christensen,[a] Espen D. Bøjesen,[a] Hermann Emerich,[d] Gavin Vaughan,[e] Simon J. L. Billinge[c,f]* and Bo B. Iversen[a]*











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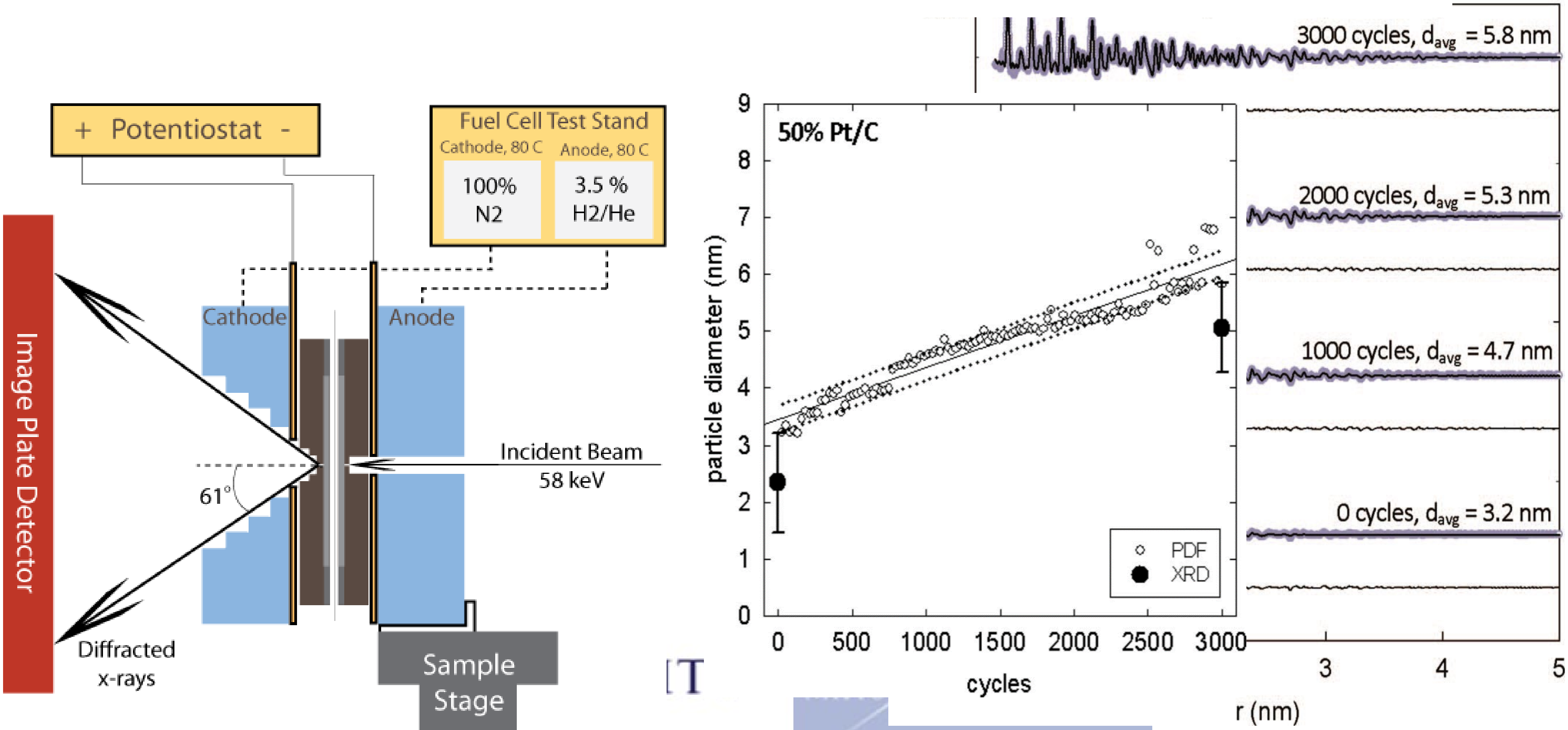
Electrochemical and Solid-State Letters, **15** (5) B72-B74 (2012)
1099-0062/2012/15(5)/B72/3/$28.00 © The Electrochemical Society

In-Situ Monitoring of Particle Growth at PEMFC Cathode under Accelerated Cycling Conditions

Erin L. Redmond,[a,*,z] Brian P. Setzler,[a,*] Pavol Juhas,[b] Simon J. L. Billinge,[b,c] and Thomas F. Fuller[a,]**

[a] *School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA*
[b] *Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York 10027, USA*
[c] *Condensed Matter and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA*



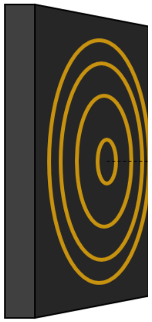
Time resolved PDF

Ultra-fast PDF

Set-Up

- **MFX** instrument at **LCLS** at **SLAC**
  - Qmax ~ 10 Å^{-1}
  - Laser delay order non-sequential
- Cooled with cryo-N_2 stream
- Sample on Kapton tape with cryogen from the side
  - Blows away ice

Rayonix MX3



$CuIr_2S_4$

Insulator
Triclinic *(P-1)*

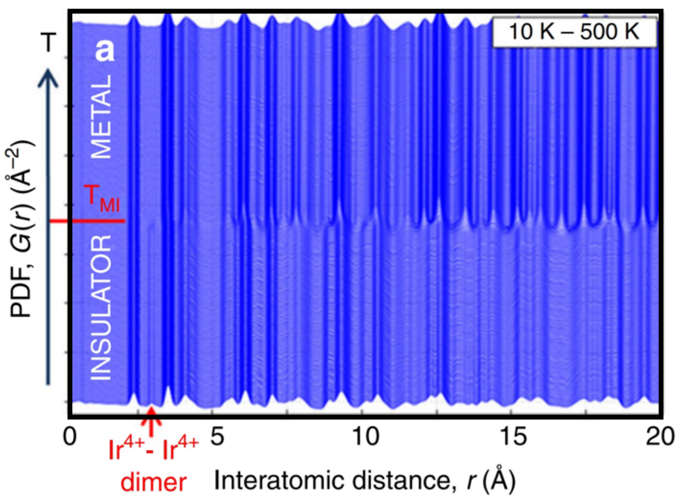
226K

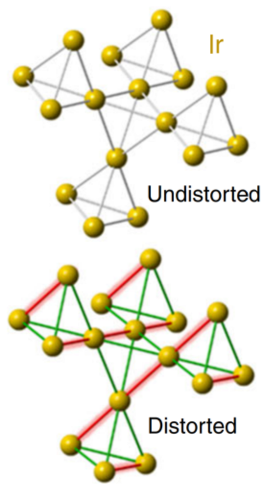
Metal
Cubic *(fm-3m)*

Low Temperature

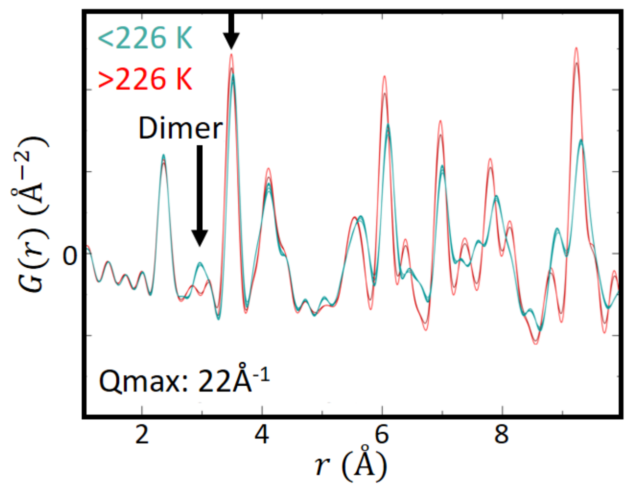
High Temperature

- Ir-Ir dimer formation in low-temperature phase
  - Clear PDF peak

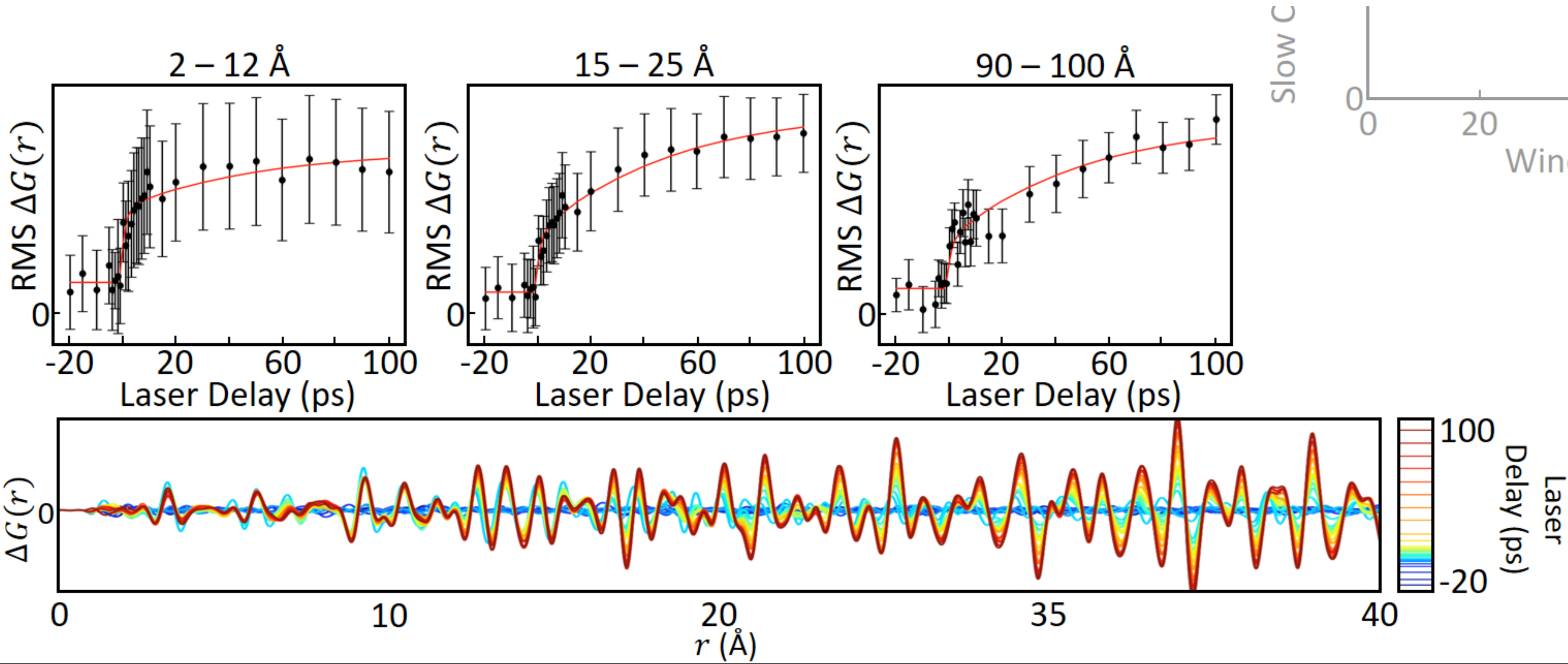




Undistorted
Ir-Ir



Nat. Comms. 10, 3638 (2019) DOI:10.1038/s41467-019-11372-w



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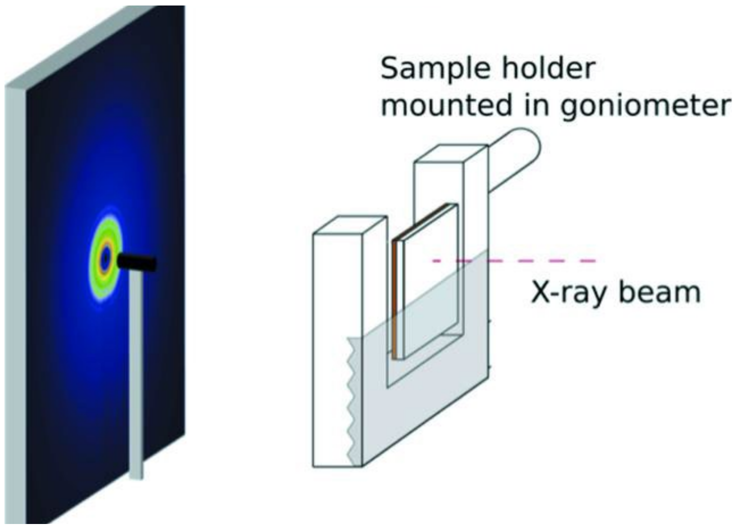
Spatially resolved PDF

Thin-film PDF and SNXM

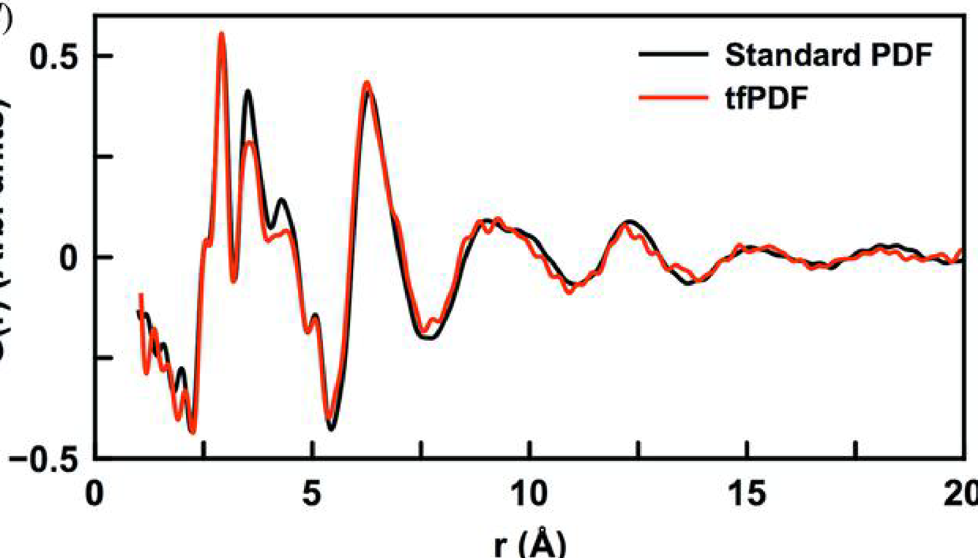
CrossMark
research papers
IUCrJ
ISSN 2052-2525
MATERIALS | COMPUTATION

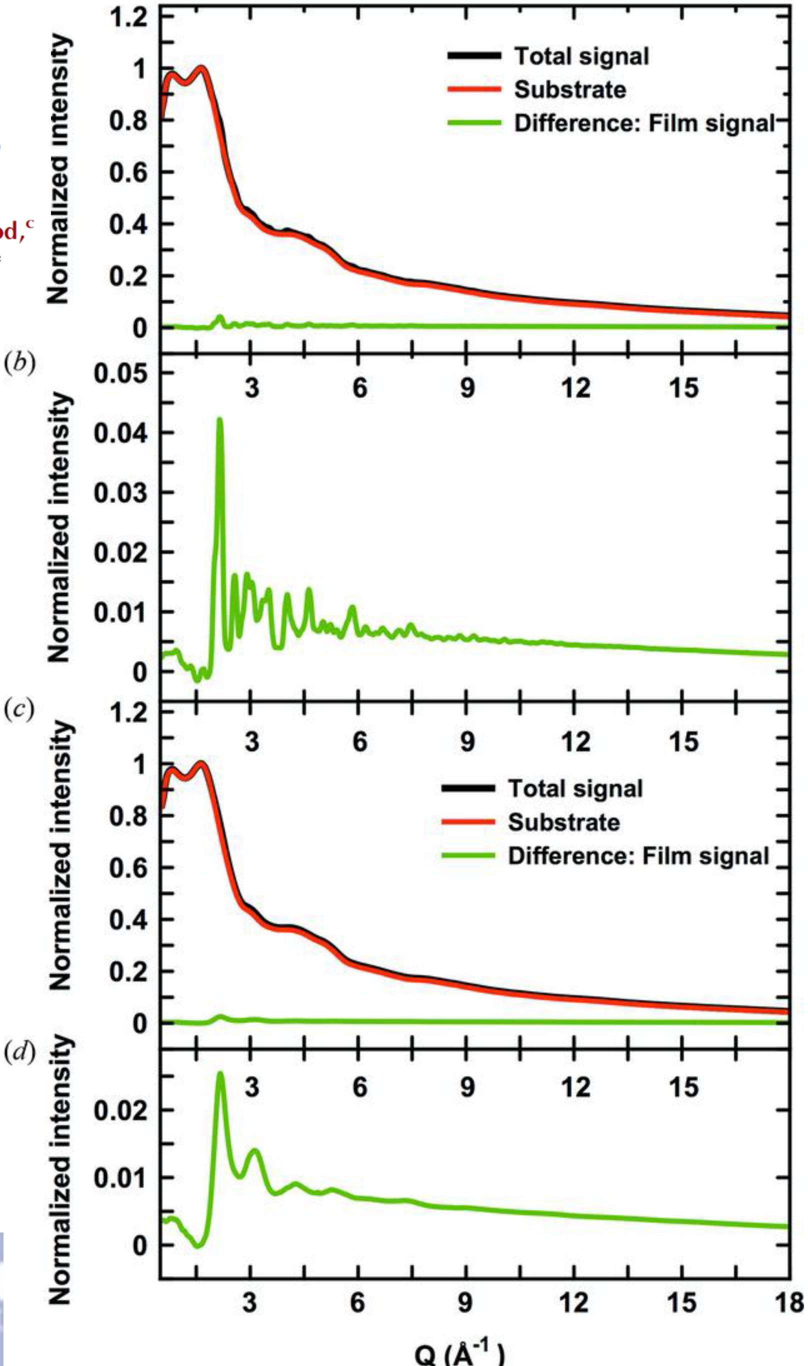
Demonstration of thin film pair distribution function analysis (tfPDF) for the study of local structure in amorphous and crystalline thin films

Kirsten M. Ø. Jensen,[a] Anders B. Blichfeld,[b] Sage R. Bauers,[c] Suzannah R. Wood,[c] Eric Dooryhée,[d] David C. Johnson,[c] Bo B. Iversen[b] and Simon J. L. Billinge[a,e]*



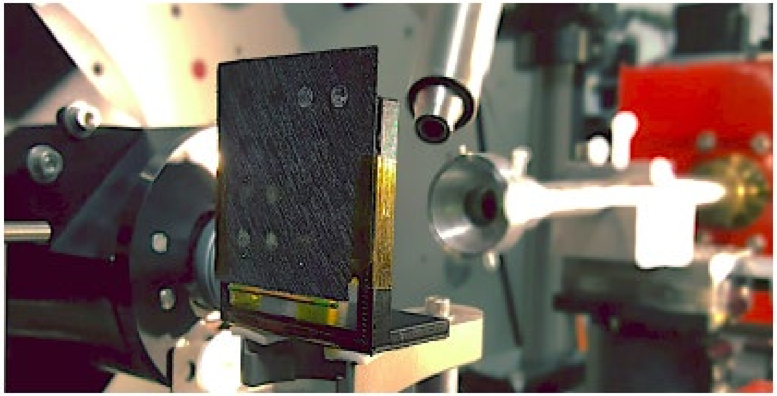
(d)

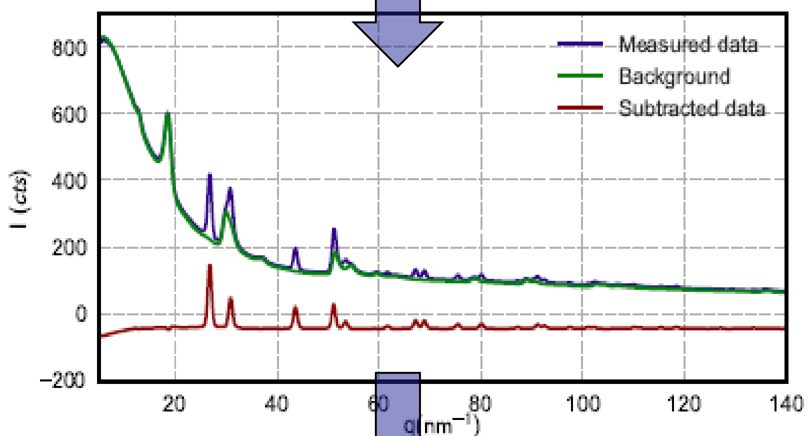


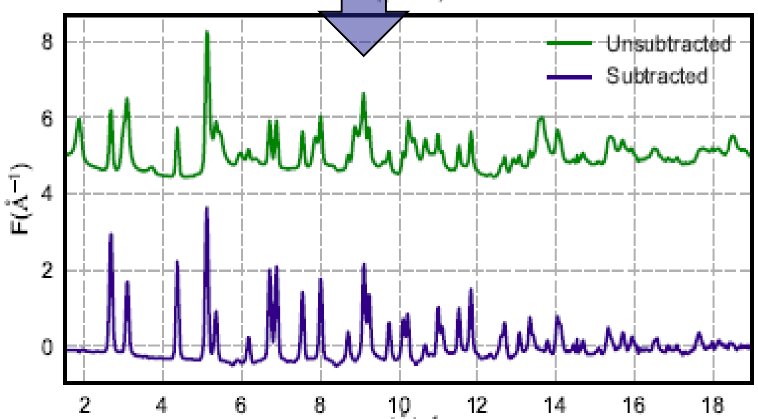


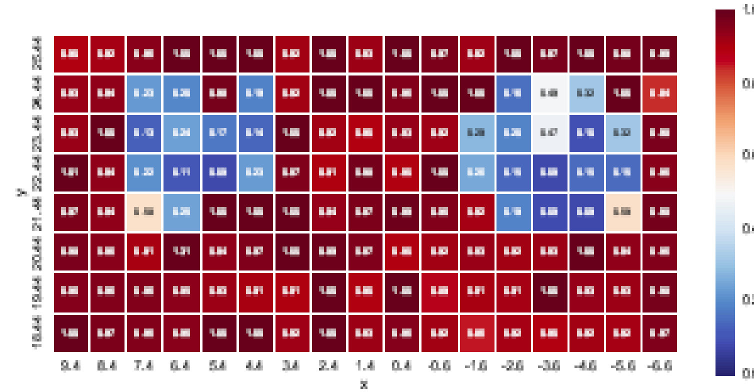
Spatially Resolved PDFs

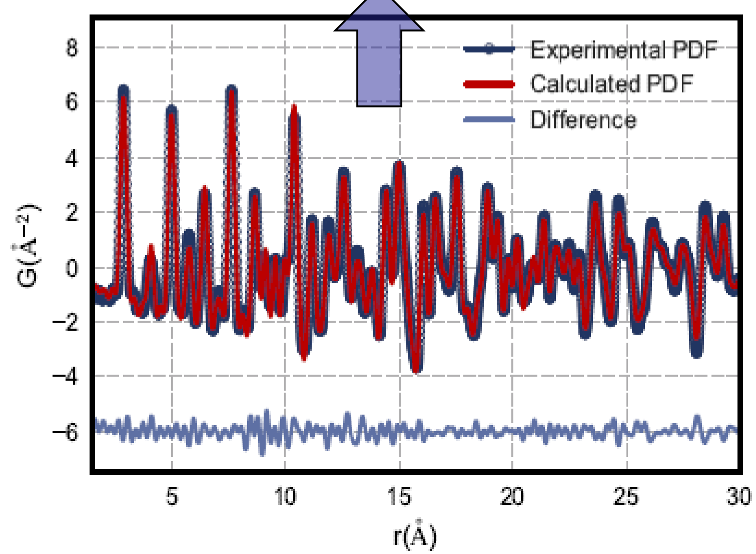
- Anton Kovyakh, Soham Banerjee, Chia Hao Liu, Tom Mallouk











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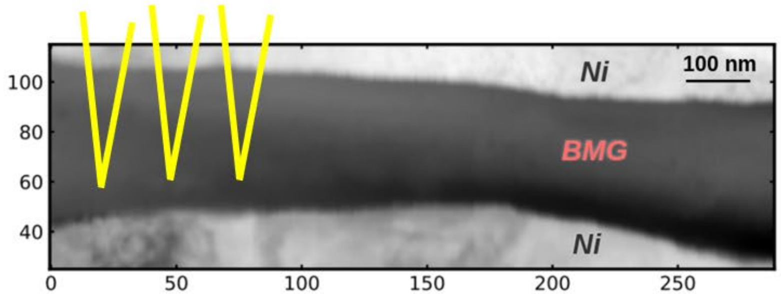
Spatially resolved PDF

SNEM

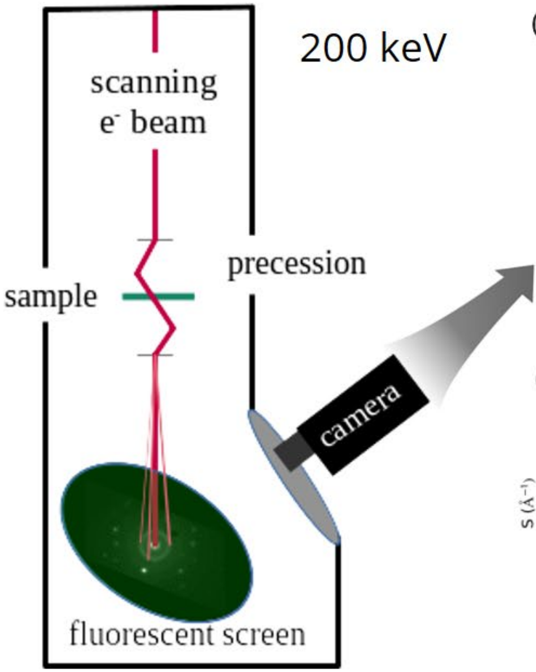
Rakita et al arXiv, Nov. *2021*, https://arxiv.org/abs/2110.03589

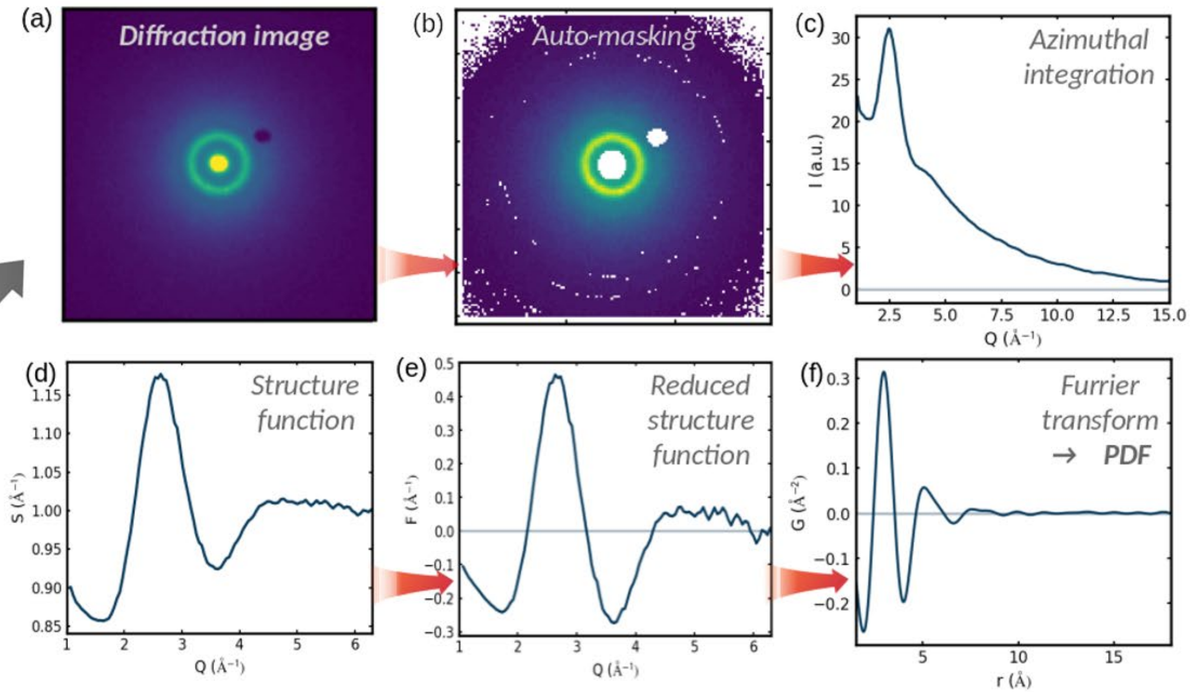


Probe: 4D-STEM

+ precession

→ to get a quasi-kinematical (x-ray-like) scattering





X 38,148 diffraction patterns

Tune once run for all

Python-based infrastructure for chaining analysis building-blocks into a coherent pipeline

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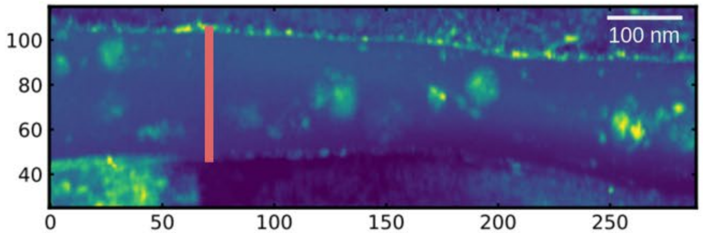
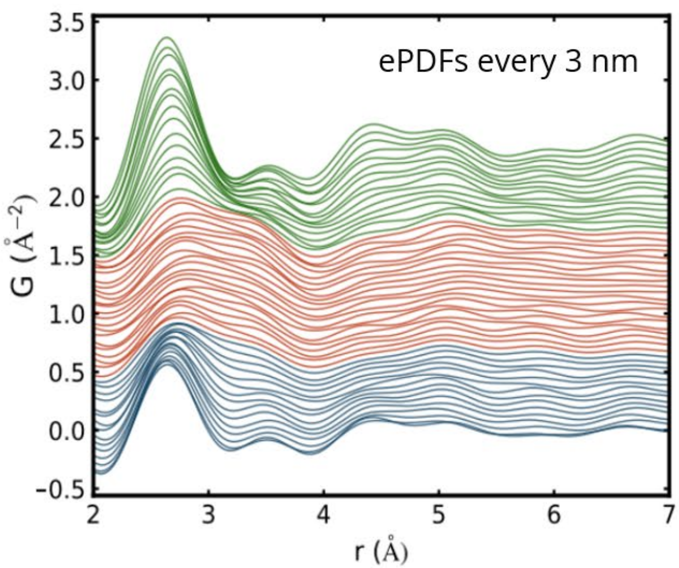
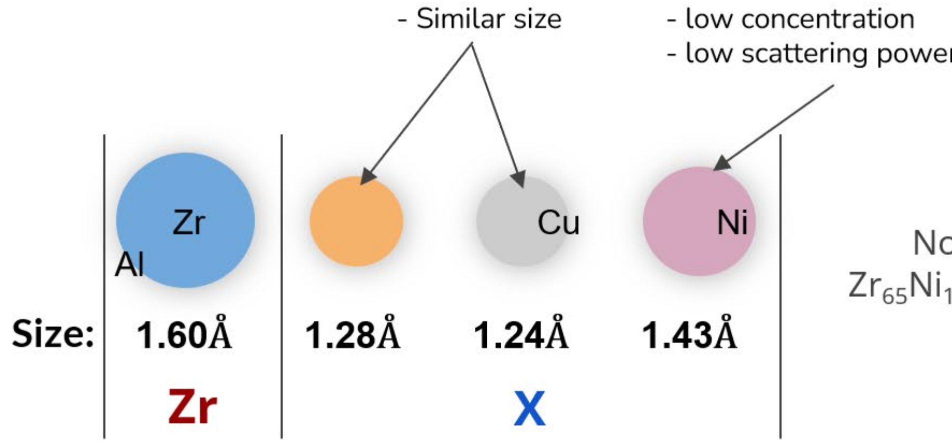
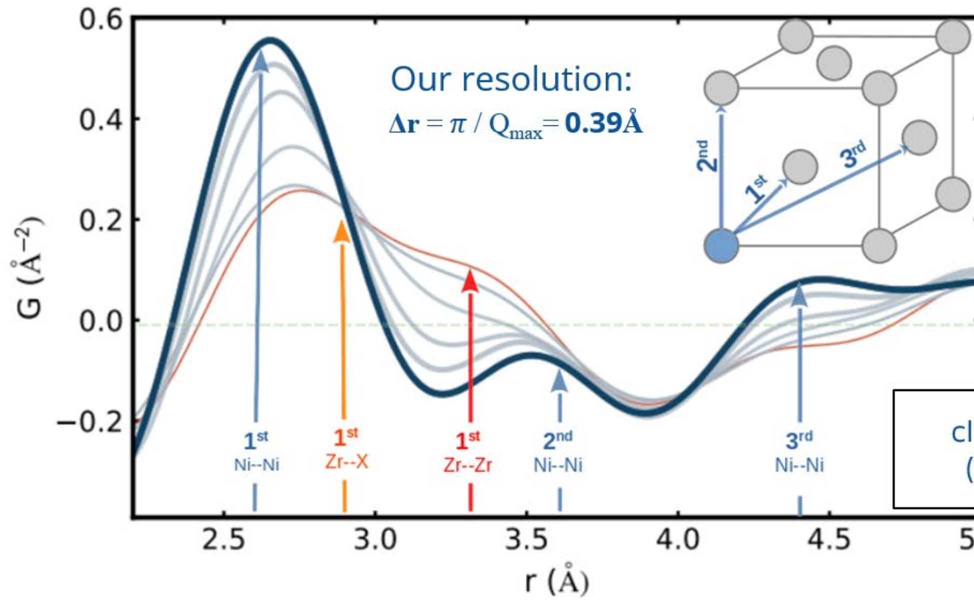
Reading the PDF's
(qualitatively)







Nominal:
$Zr_{65}Ni_{10}Cu_{17.5}Al_{7.5}$



close-packed
(fcc) + 0.1Å

PDF tomography (ctPDF)

nature COMMUNICATIONS

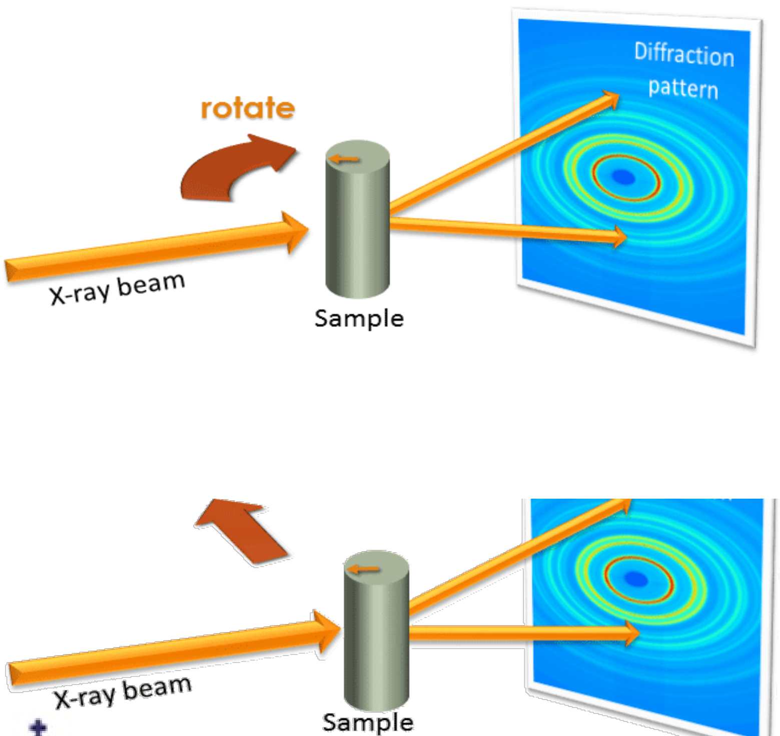
ARTICLE

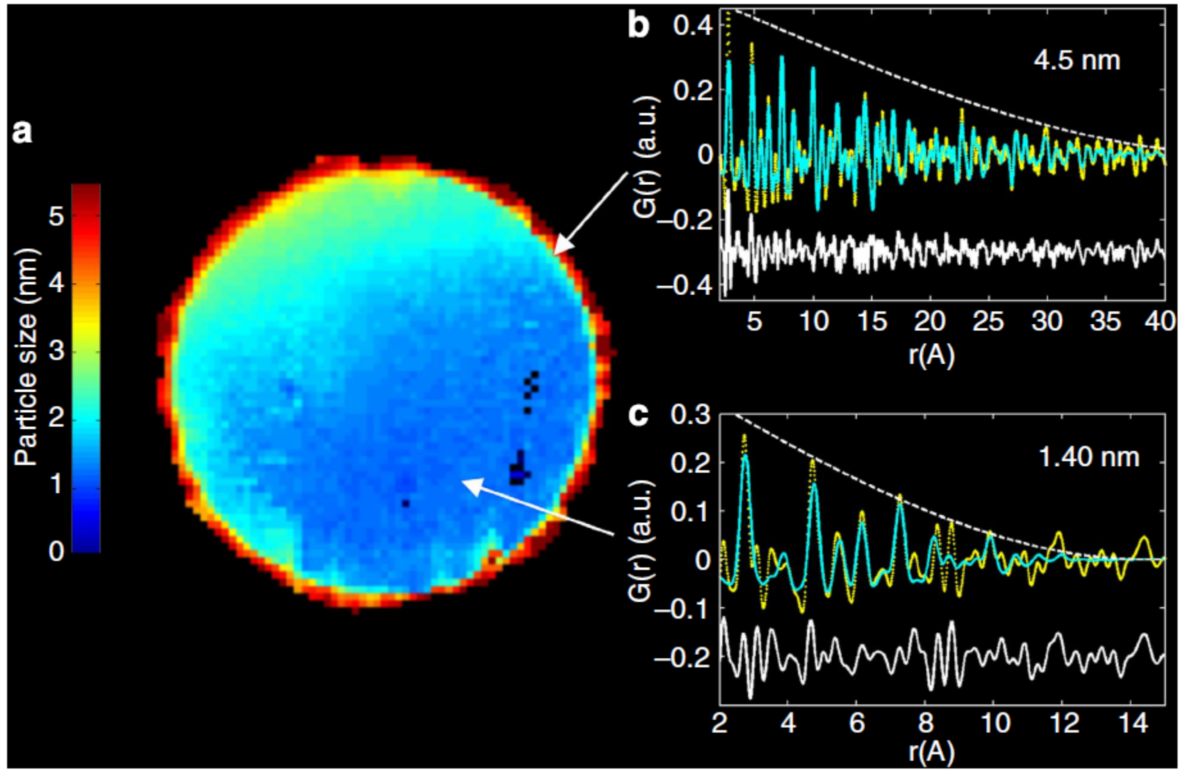
Received 26 Apr 2013 | Accepted 3 Sep 2013 | Published 30 Sep 2013

DOI: 10.1038/ncomms3536

Pair distribution function computed tomography

Simon D.M. Jacques[1,2], Marco Di Michiel[3], Simon A.J. Kimber[3], Xiaohao Yang[4], Robert J. Cernik[1], Andrew M. Beale[2,5,6] & Simon J.L. Billinge[4,7]





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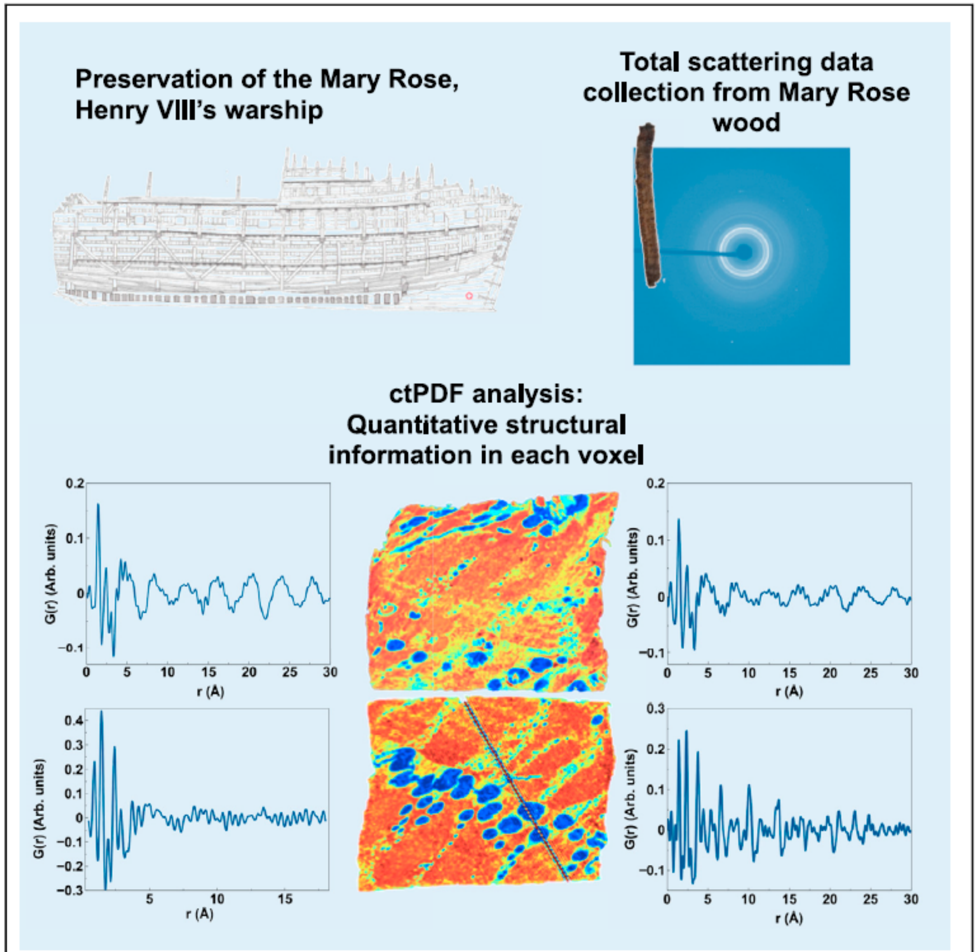
Matter

CellPress

Article

Location and characterization of heterogeneous phases within *Mary Rose* wood



Kirsten M.Ø. Jensen, Esther Rani Aluri, Enrique Sanchez Perez, ..., Eleanor J. Schofield, Simon J.L. Billinge, Serena A. Cussen

s.cussen@sheffield.ac.uk (S.A.C.)
kirsten@chem.ku.dk (K.M.Ø.J.)
e.schofield@maryrose.org (E.J.S.)
sb2896@columbia.edu (S.J.L.B.)

Highlights

Wood from the *Mary Rose* is characterized with computed tomography total scattering

Polyethylene glycol from previous conservation treatments is identified and mapped

Five-nanometer zinc sulfide nanoparticles are identified in the waterlogged wood

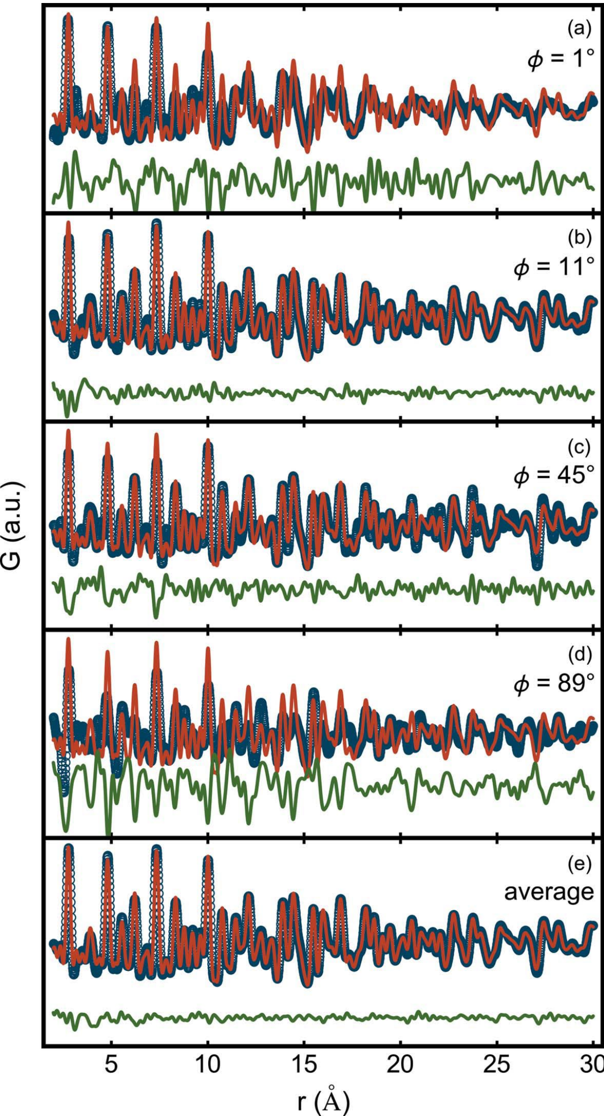
Total scattering analysis shows position-dependent structure of the nanoparticles

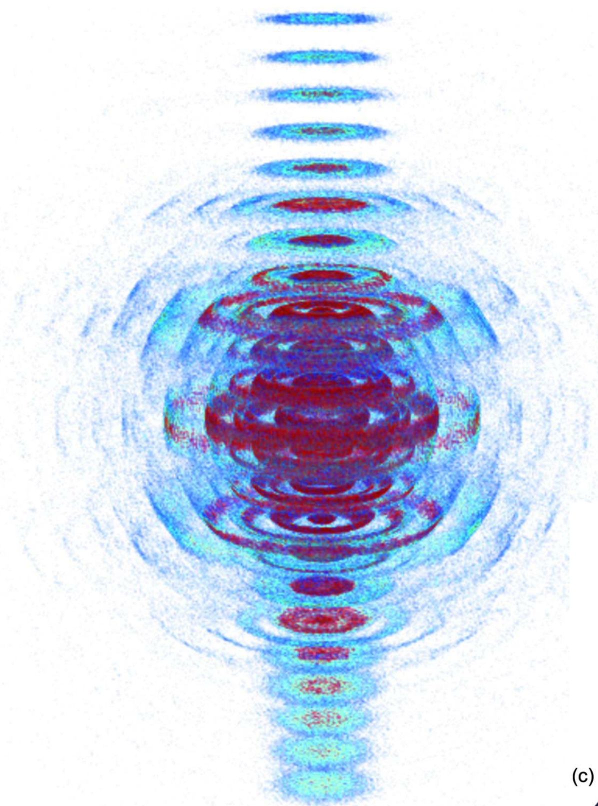
Crystalline Texture

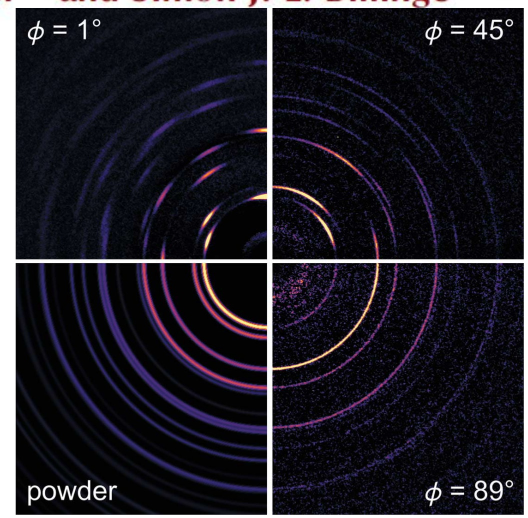
IUCrJ
ISSN 2052-2525
MATERIALS | COMPUTATION

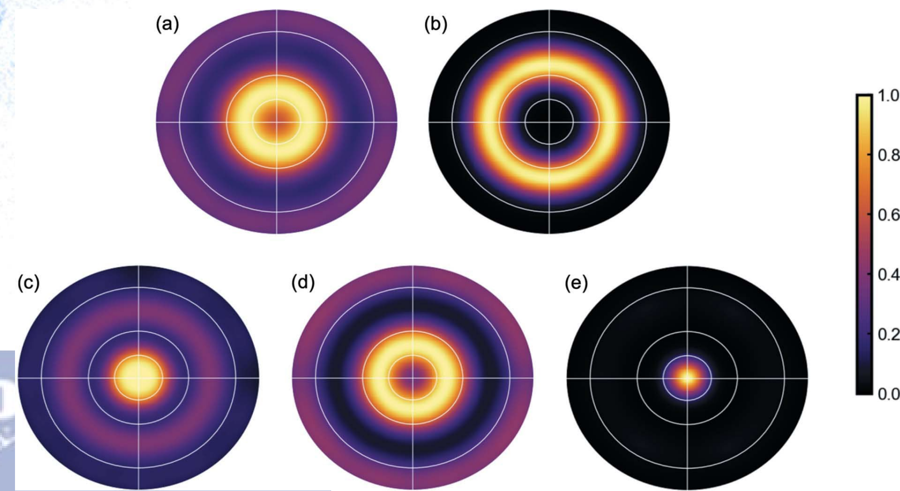
Real-space texture and pole-figure analysis using the 3D pair distribution function on a platinum thin film

Sani Y. Harouna-Mayer,[a,b] Songsheng Tao,[c] ZiZhou Gong,[c] Martin v. Zimmermann,[d] Dorota Koziej,[a,b] Ann-Christin Dippel[d]* and Simon J. L. Billinge[c,e]*

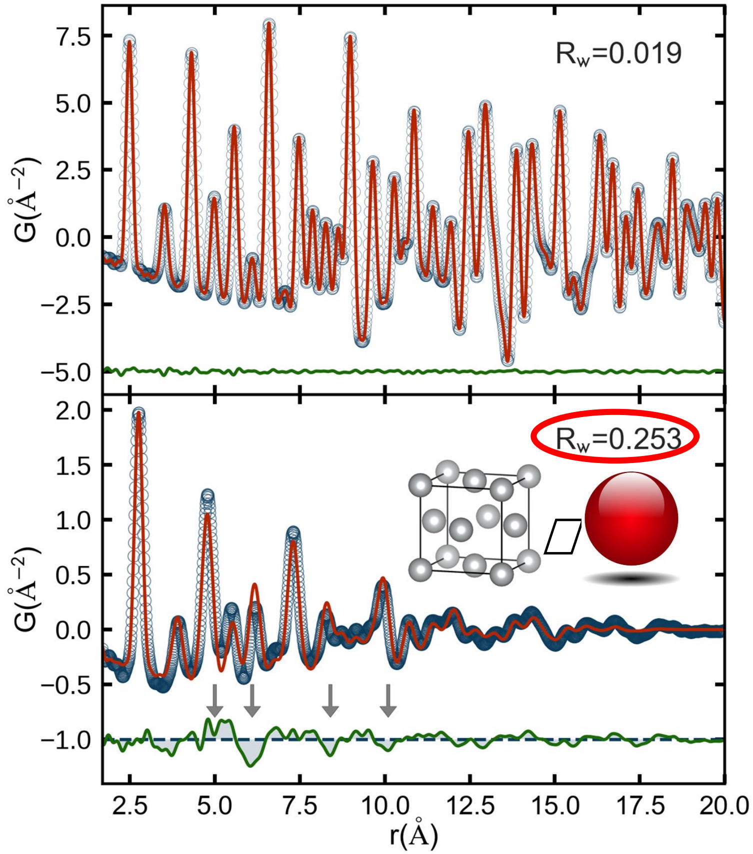




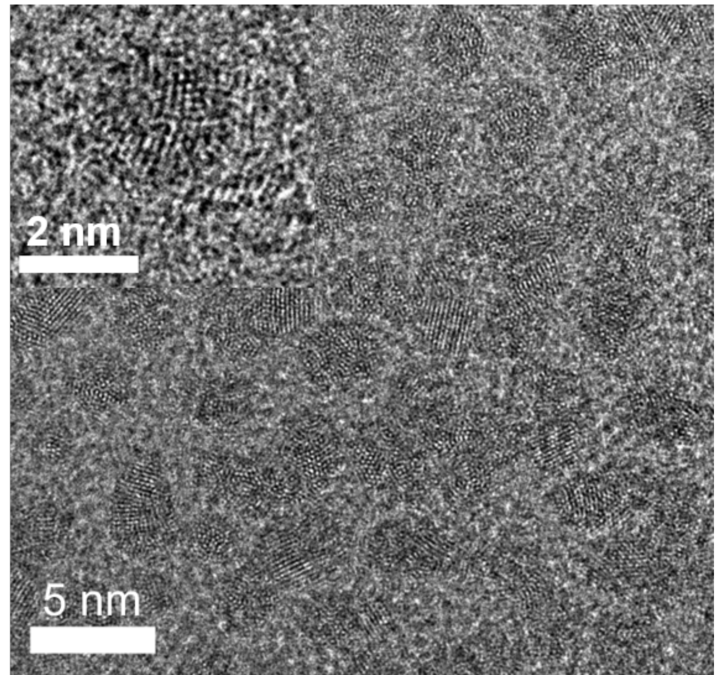


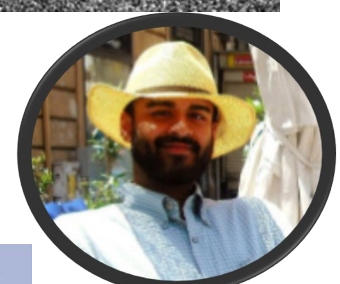


High throughput data analysis and modeling methods



~3 nm Pd nanoparticles





Banerjee, S., et al. Acta Cryst A 76.
https://doi.org/10.1107/S2053273319013214

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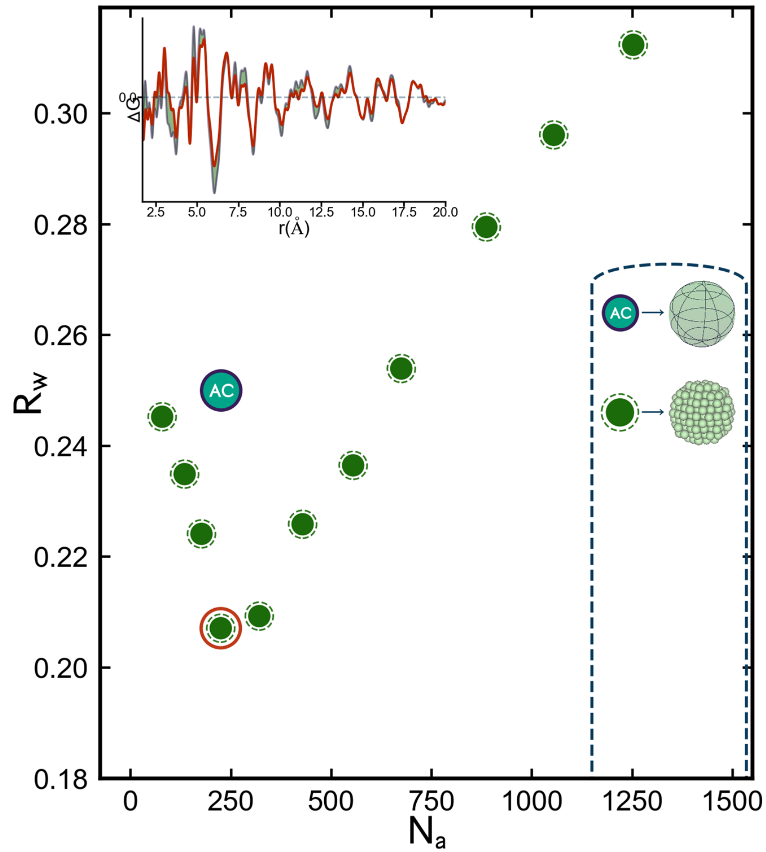

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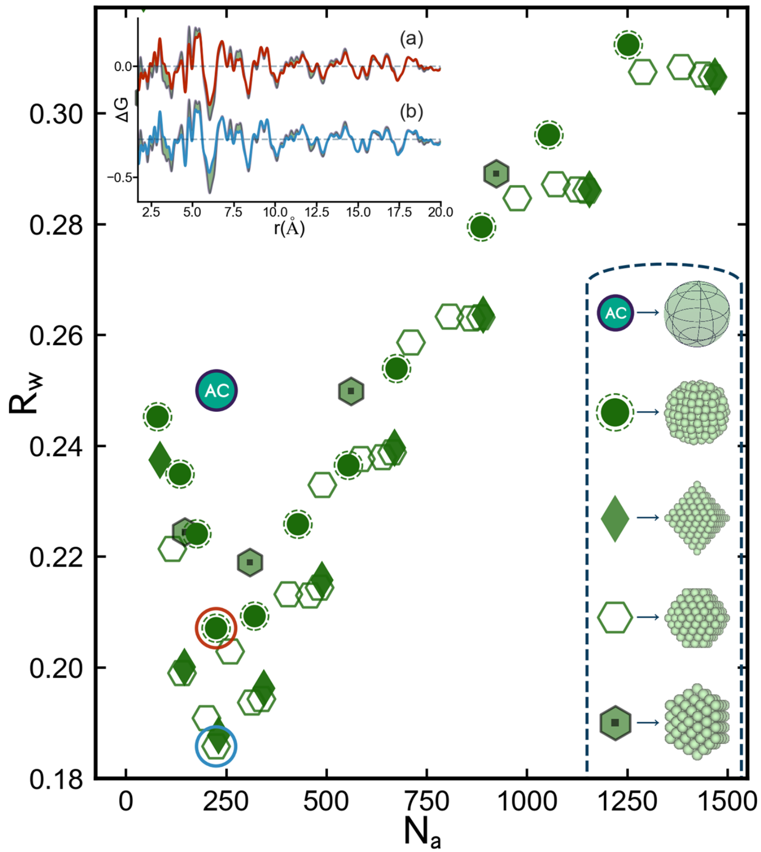

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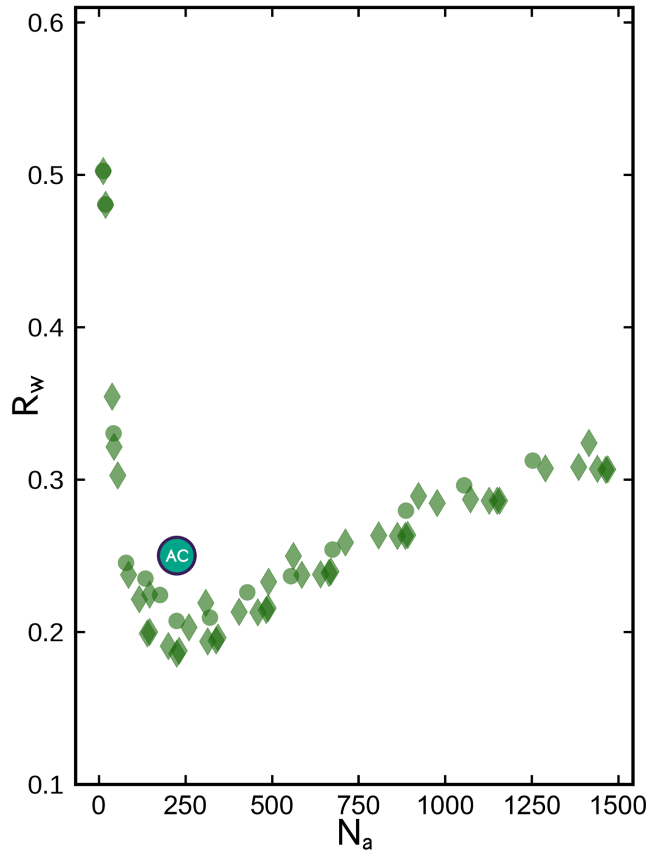
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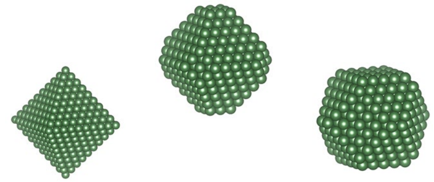

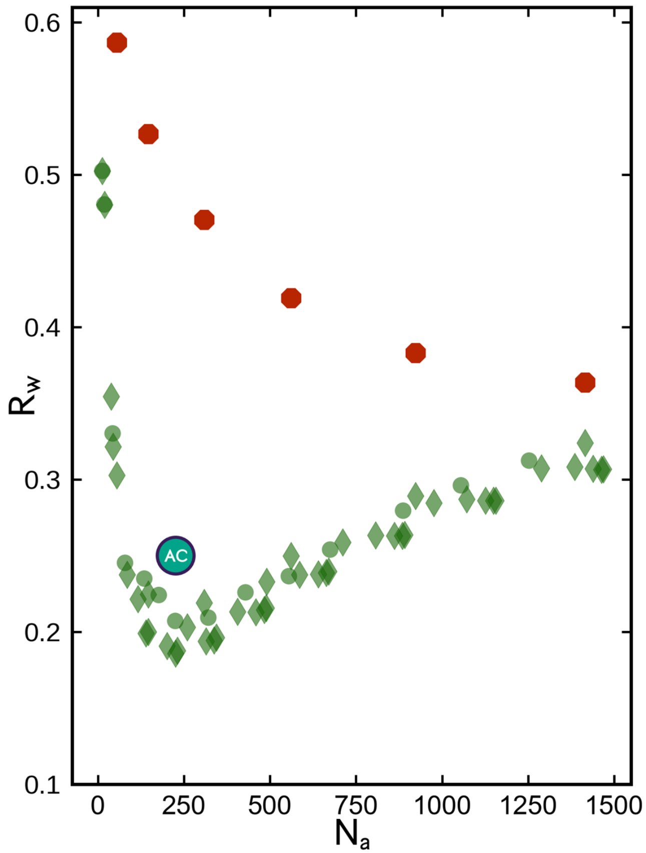
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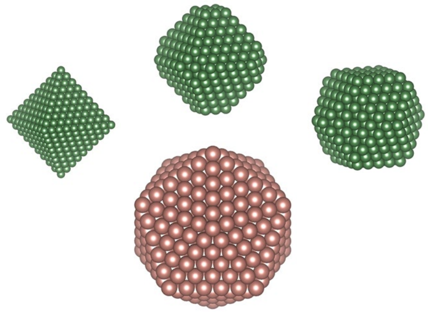

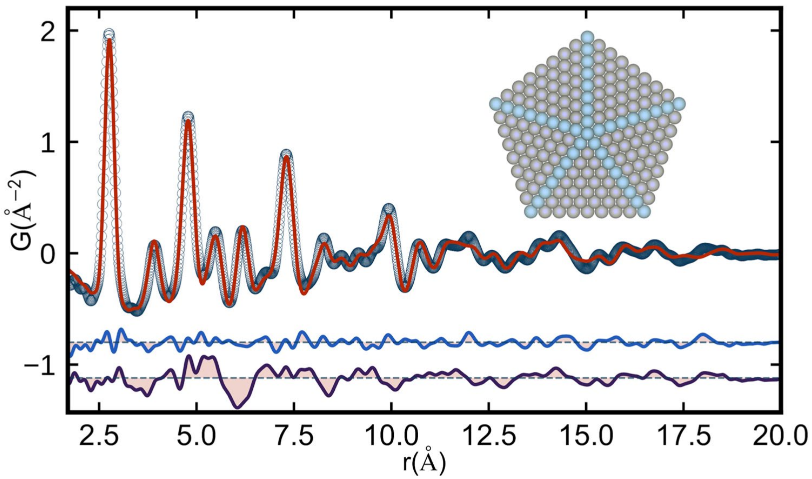

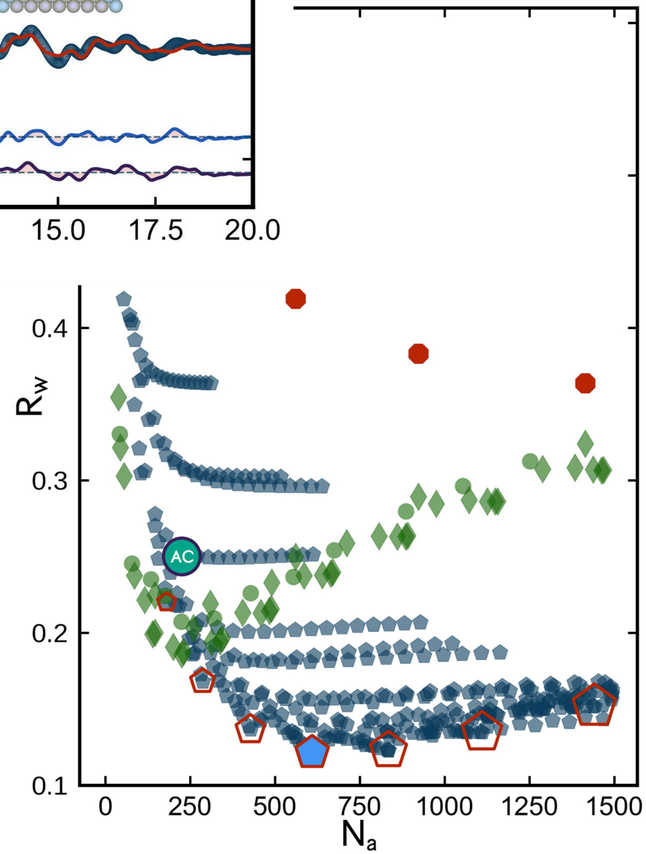

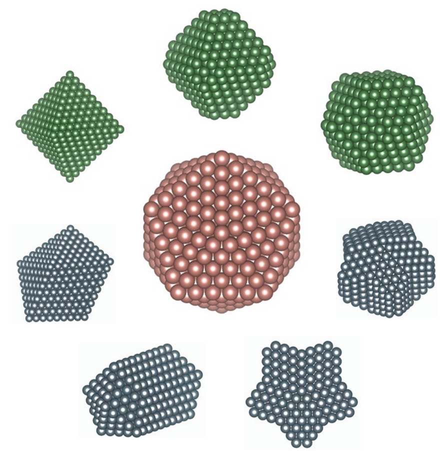

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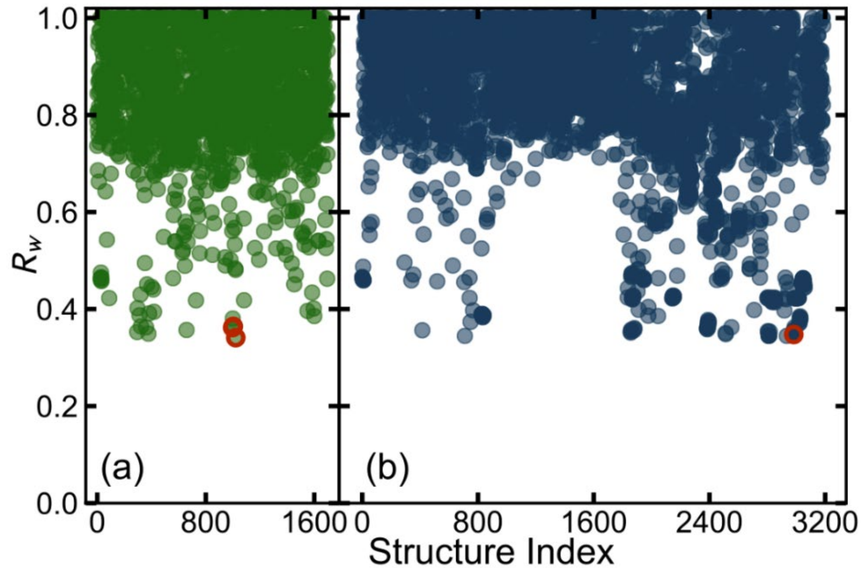
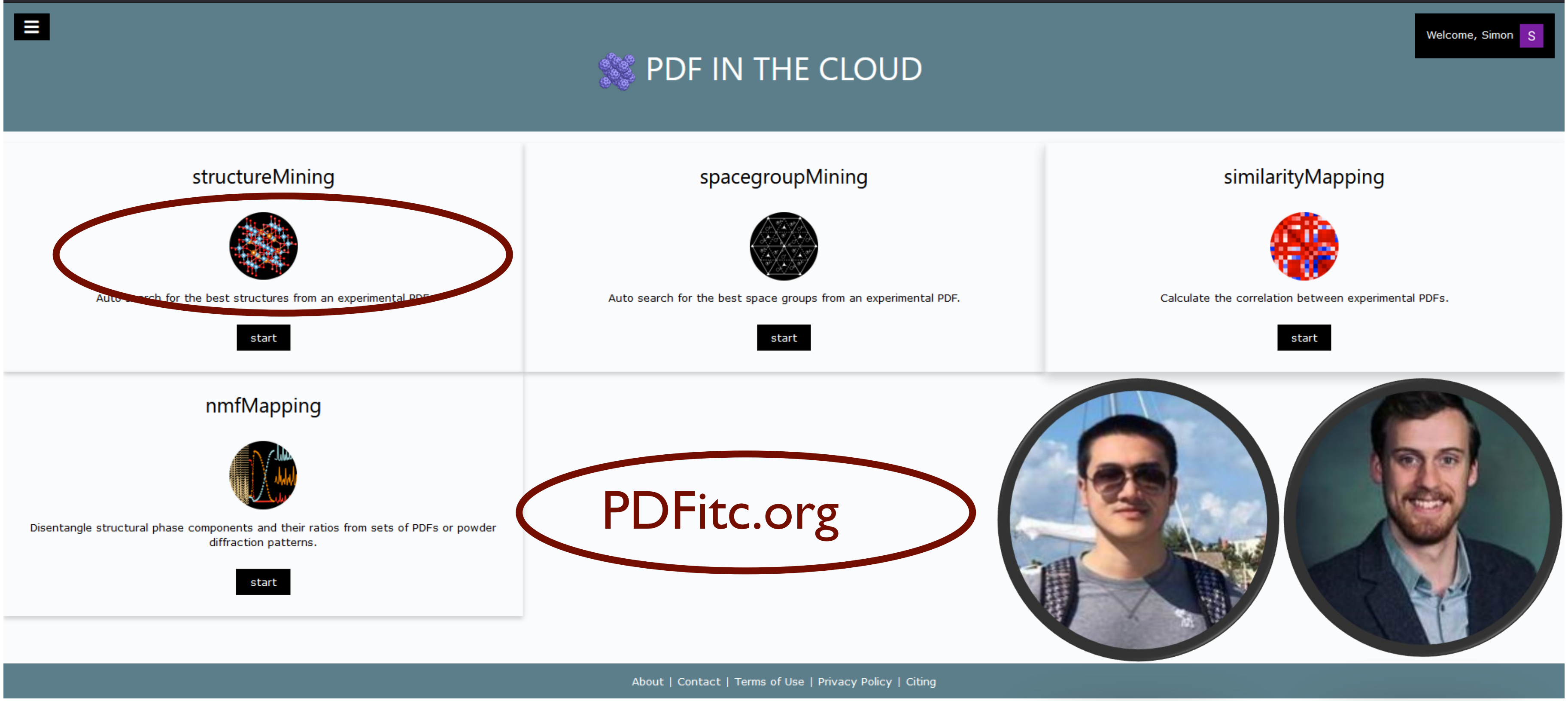
With databases you can directly do data mining: structureMining



- Upload a PDF and some basic compositional information and search for close matches, e.g., $NaFeSi_2O_6$ nanowire date
  - Structure-mining found the same model as in prior work, MPD No. 1003 ($NaFeSi_2O_6$) and COD No. 2983 ($NaFeSi_2O_6$), s.g.: C 2/c.
  - It also returns some structures with space group C 2, such as MPD No. 998 ($Na_{0.83}FeSi_2O_6$), which may be viewed as a very similar structure but with a lowered symmetry and deficient atoms at some sites
  - It also returns some structures substituting at Na or Fe sites by other elements. For example, MPD No. 1021 ($NaGaSi_2O_6$).



- Web platform developed as part of an NSF funded project, but nmfMapping App is a GENESIS product (Long Yang and Zach Thatcher)
- Upload a set of data (powder diffraction or PDF), get back the structure/space-group/NMF components and weights/Pearson matrix

Upload a PDF, click go

PDF IN THE CLOUD

structureMining

Given a measured (or calculated) PDF, structureMining will search databases to find the best structures to fit it.

Please see the strucureMining paper for more information. Please cite the structureMining paper if this helps you get a publishable result:
L. Yang, P. Juhás, M. W. Terban, M. G. Tucker, and S. J. L. Billinge. Structure-mining: screening structure models by automated fitting to the atomic pair distribution function over large numbers of models. *Acta Crystallogr. A.* (2020). 76(3), 395-409. doi:10.1107/S2053273320002028

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Optional Parameter:

Type of PDF: ○ Experimental ○ Simulated

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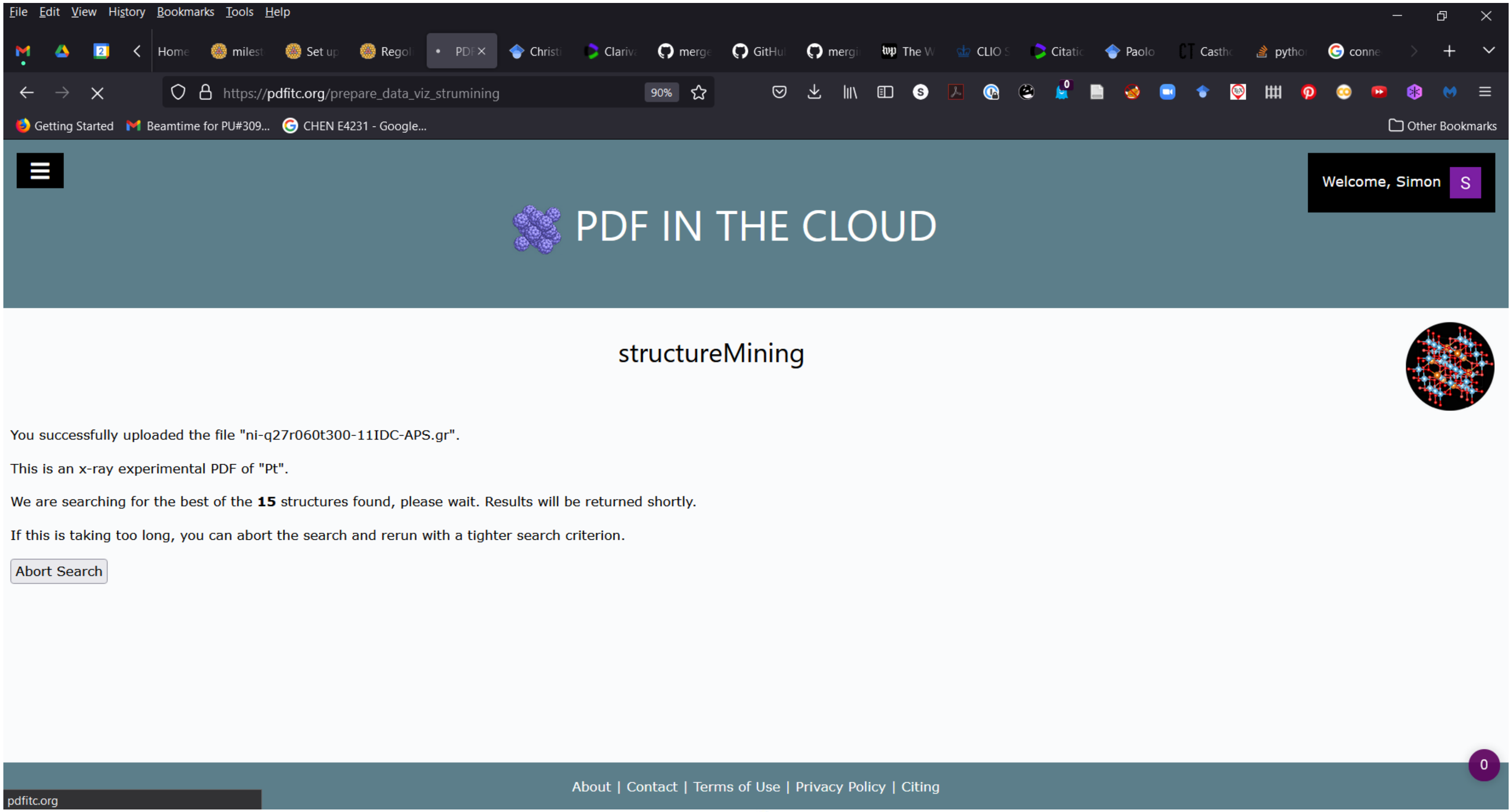

Get your CIFs back

structureMining

Results

SM found total 15 structures and 0 structures with weighted profile agreement factor, Rw < 0.5. Download All Results

Expand Table

	rw	formula	space_group	db	db_id	ref	download
0	0.985338	Pt	Fm-3m	COD	1011114	Uspenski. Zeitschrift fuer Physik. 16 (1923) 215--227	
1	0.986745	Pt	Fm-3m	COD	2104023	Shiraki. Acta Crystallographica Section B. 59 (2003) 701--708	
2	0.987596	Pt	Fm-3m	MPD	mp-126	Yan et al. International Journal of Materials Research. 102 (2011) 381-388	
3	0.987993	Pt	Fm-3m	COD	2104029	Shiraki. Acta Crystallographica Section B. 59 (2003) 701--708	
4	0.989126	Pt	Fm-3m	COD	2104026	Shiraki. Acta Crystallographica Section B. 59 (2003) 701--708	
5	0.993182	Pt	Fm-3m	COD	4334349	Ochi. Inorganic Chemistry. 52 (2013) 3985--3989	
6	0.993182	Pt	Fm-3m	COD	9008480	Wyckoff. Crystal Structures. 1 (1963) 7--83	
7	0.993183	Pt	Fm-3m	COD	1011113	Davey. Physical Review (1,1893-132,1963/141,1966-188,1969). 25 (1925) 753--761	

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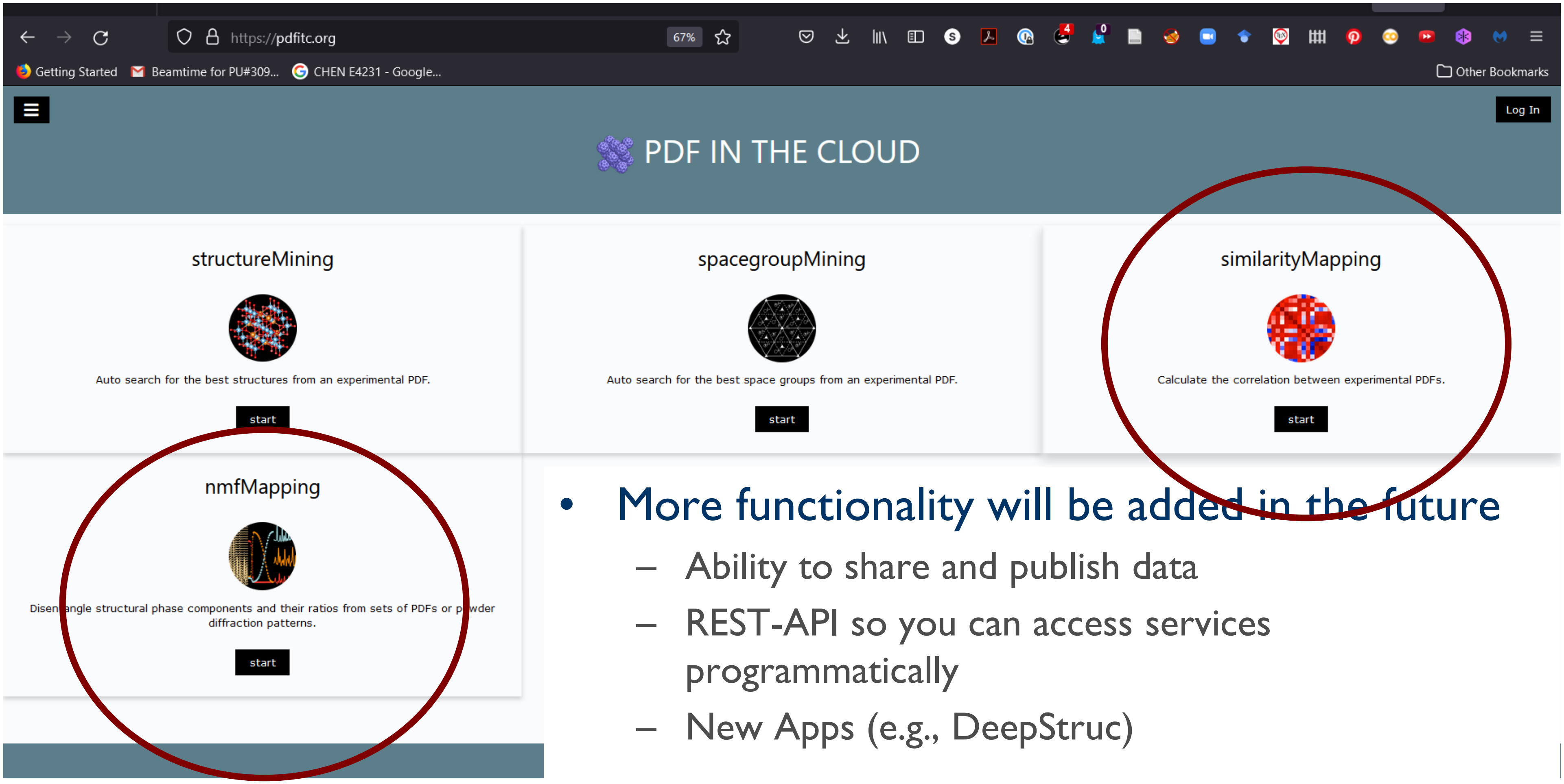
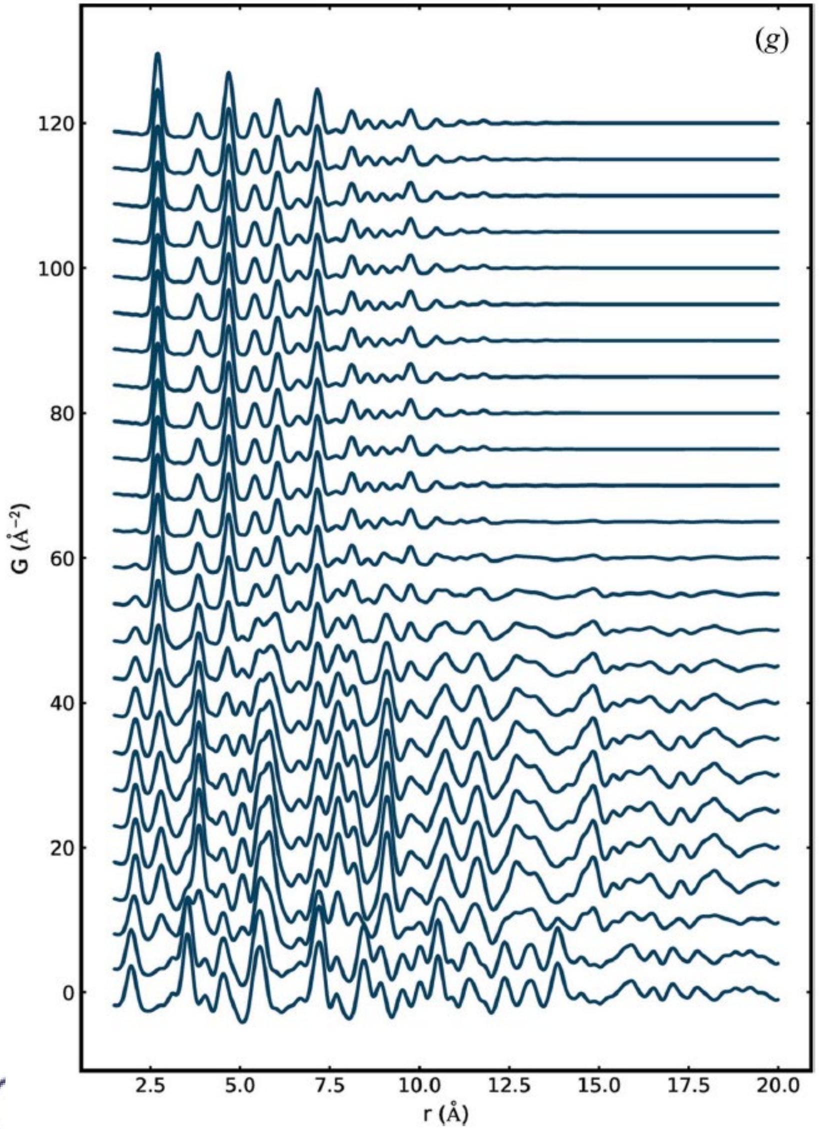
Pdfitc.org will do this for you with no programming experience



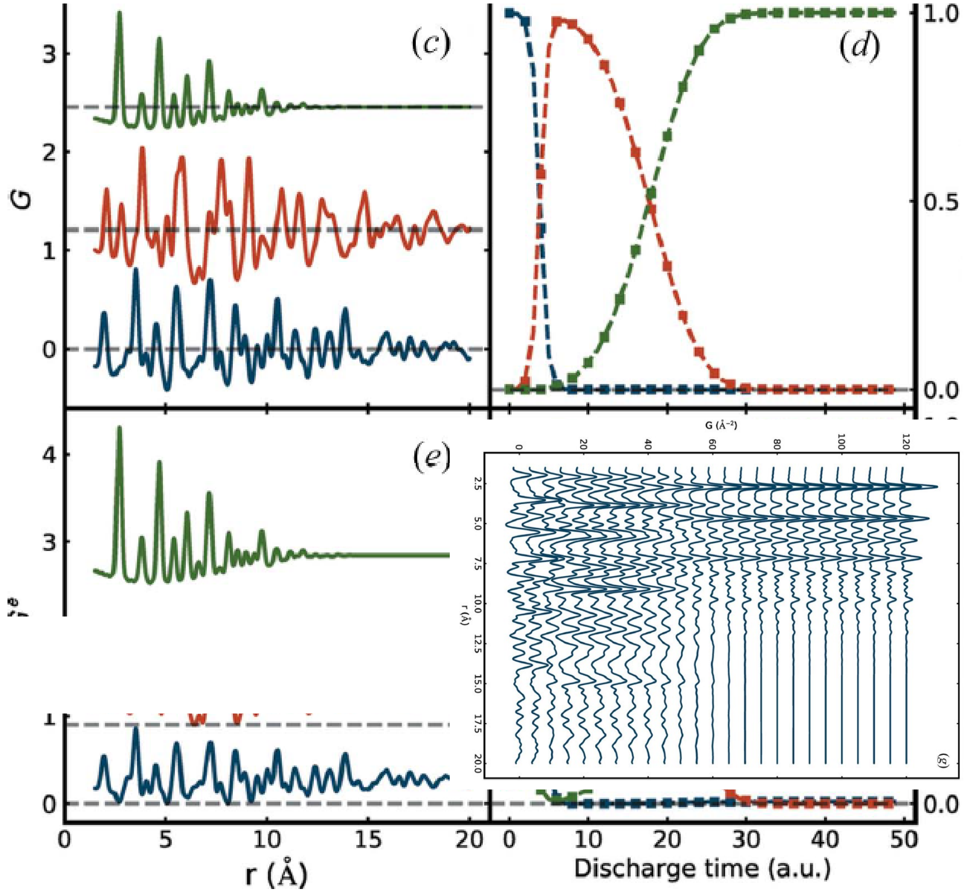
- More functionality will be added in the future
  - Ability to share and publish data
  - REST-API so you can access services programmatically
  - New Apps (e.g., DeepStruc)
  - ...

Extracting meaning from large sets of data



- E.g., 200 datasets from an in situ battery discharge experiment
- Small number of chemical species are coming and going
- Applied Math knows no chemistry, but unsupervised learning methods can find the signals (components) of the different chemical components automatically

Non negative matrix factorization (NMF)



- Collaboration with Karina Chapman group
- Ground truth
  1. Simulate 3 PDFs of 3 phases of a battery materials
  2. Stipulate how they appear and disappear with time
  3. Make PDFs that are linear combinations with these weights
  4. Run NMF on them
- Liu, SJLB, et al., J. Appl. C (2021) 10.1107/S160057

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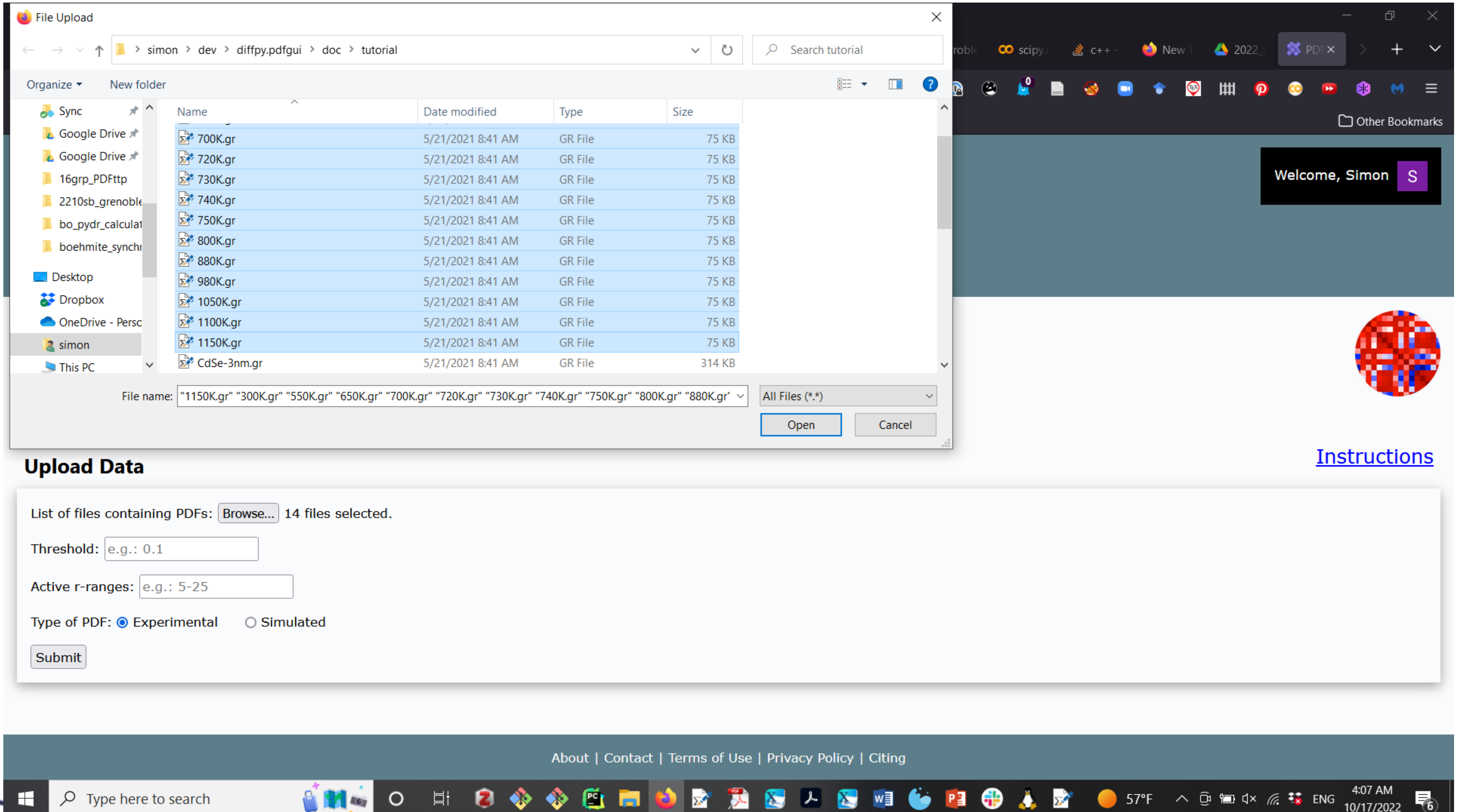
Pearson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Results

Pearson calculated the following results with no threshold and an r-range over the entire range.

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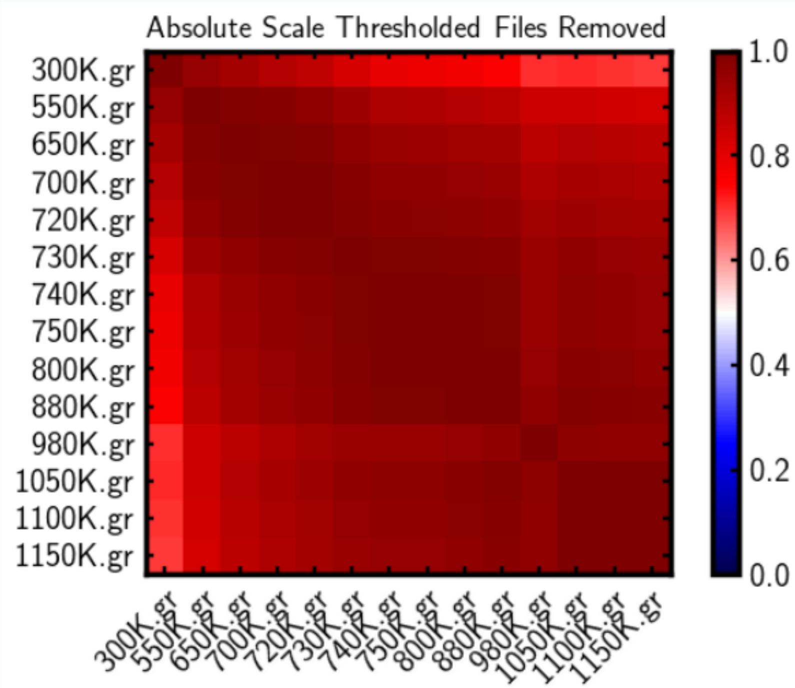

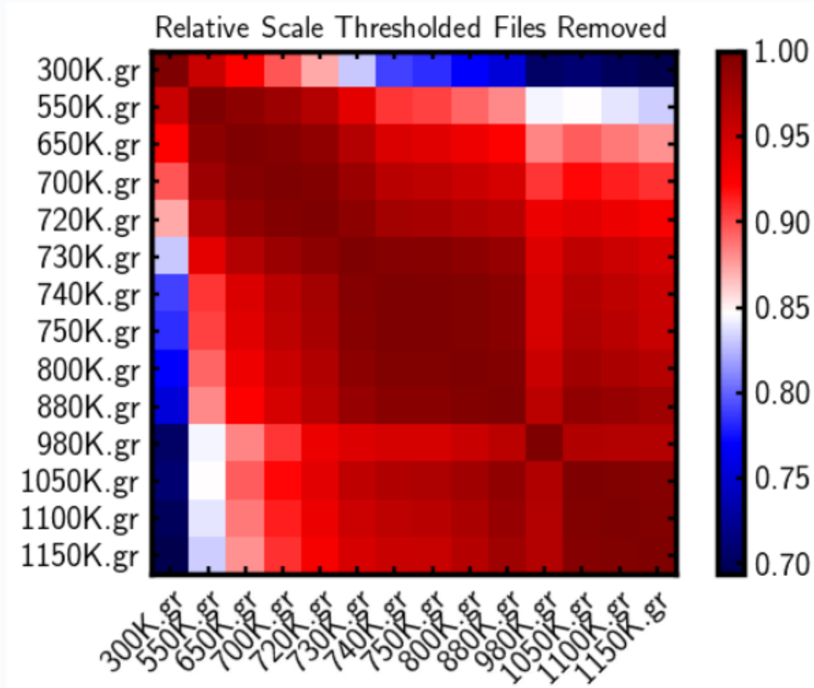

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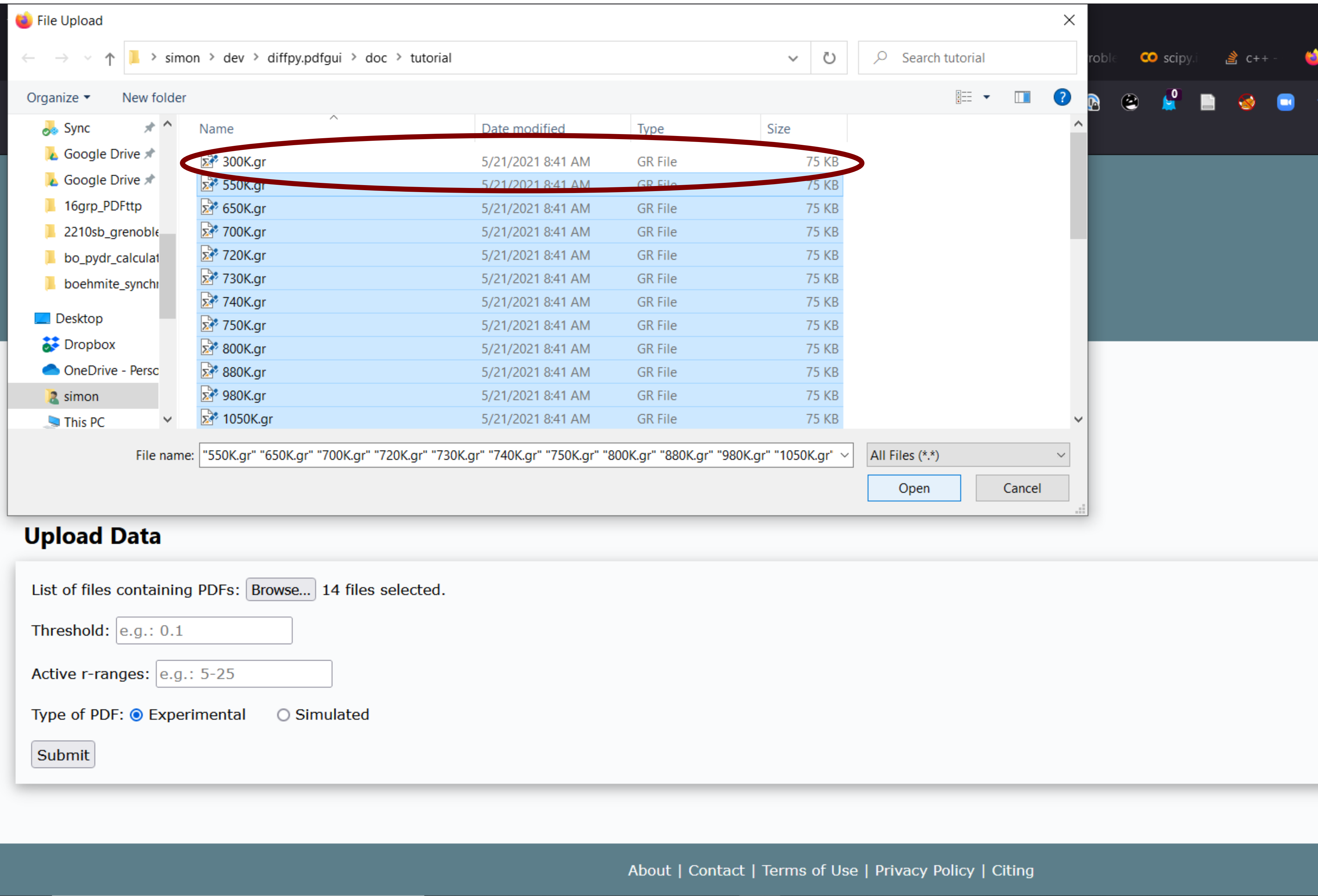
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Active r-ranges: e.g.: 5-25
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Results

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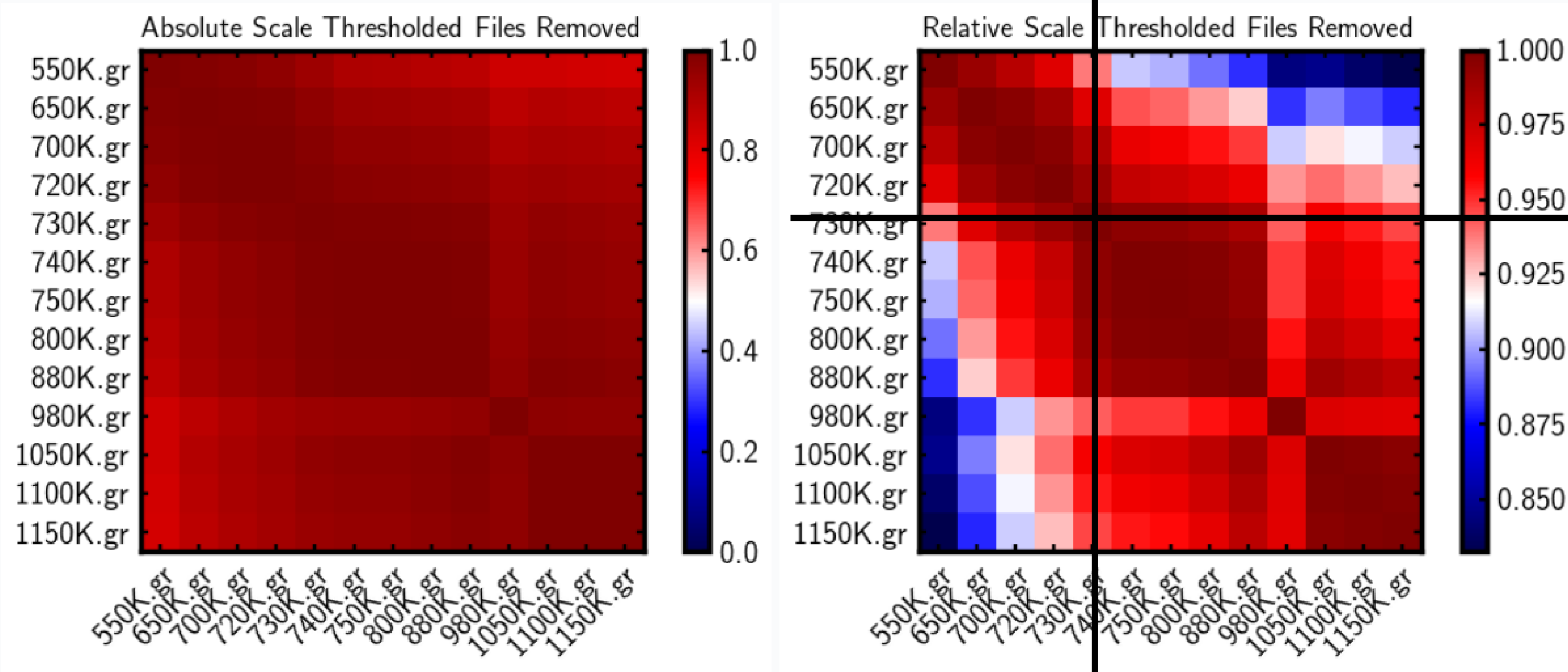

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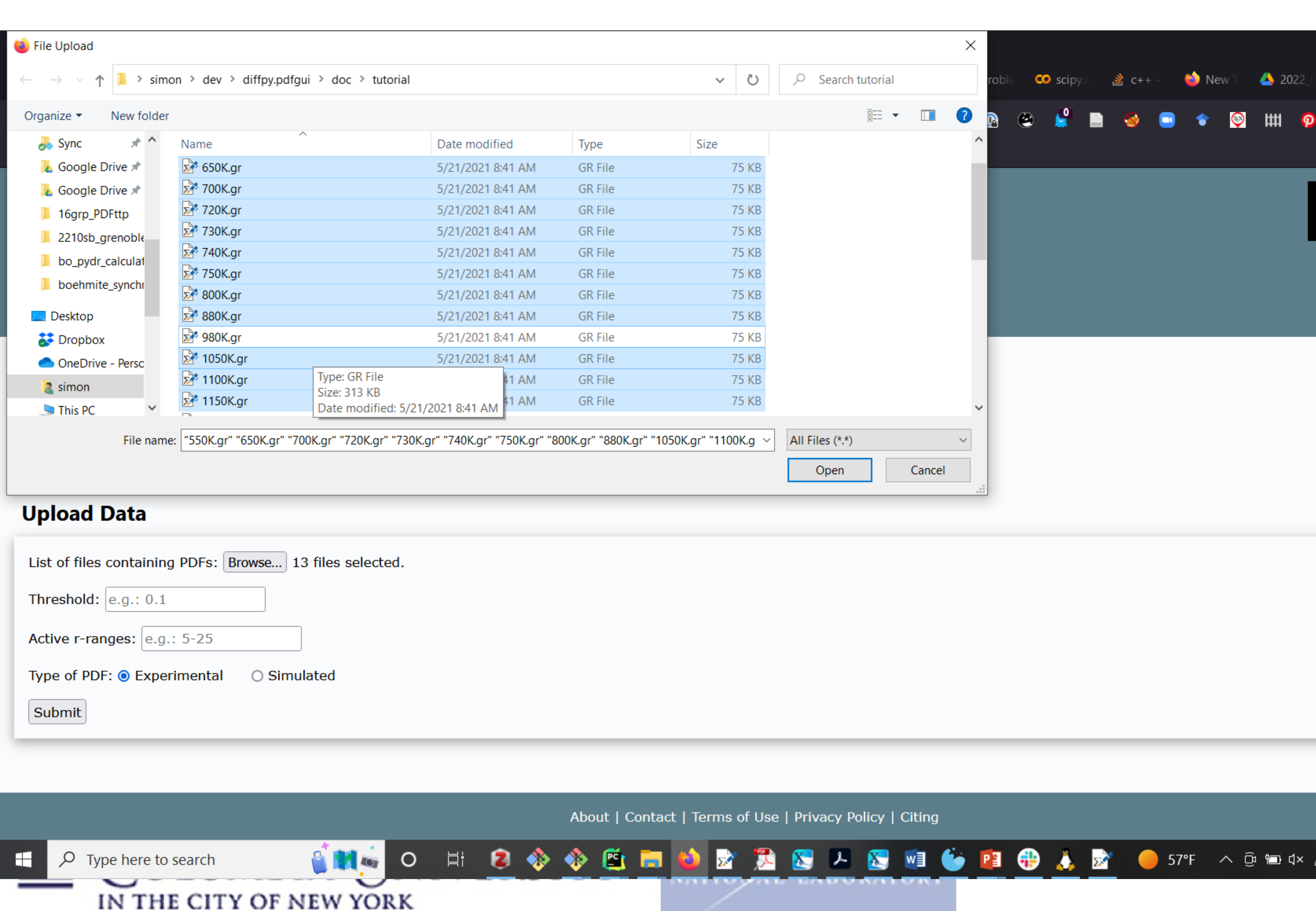
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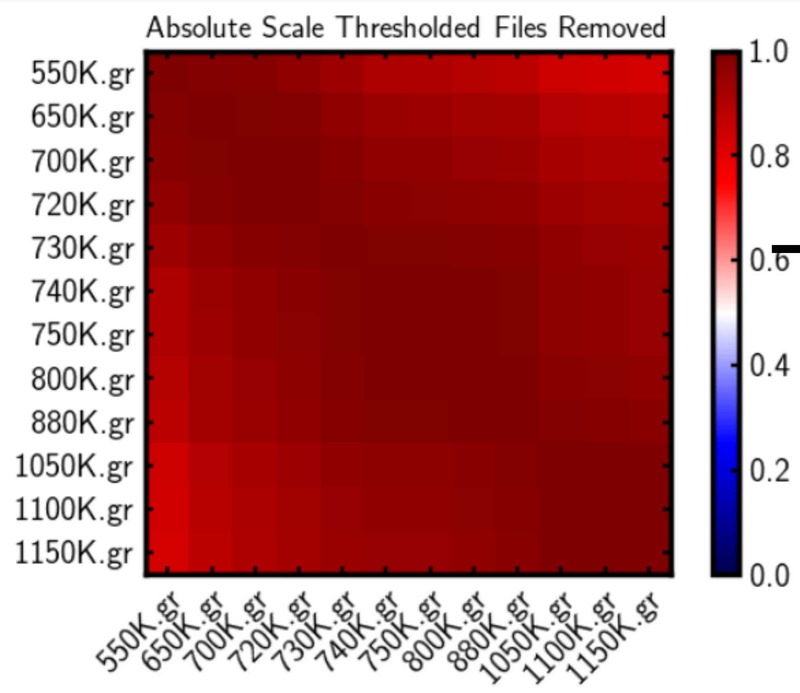

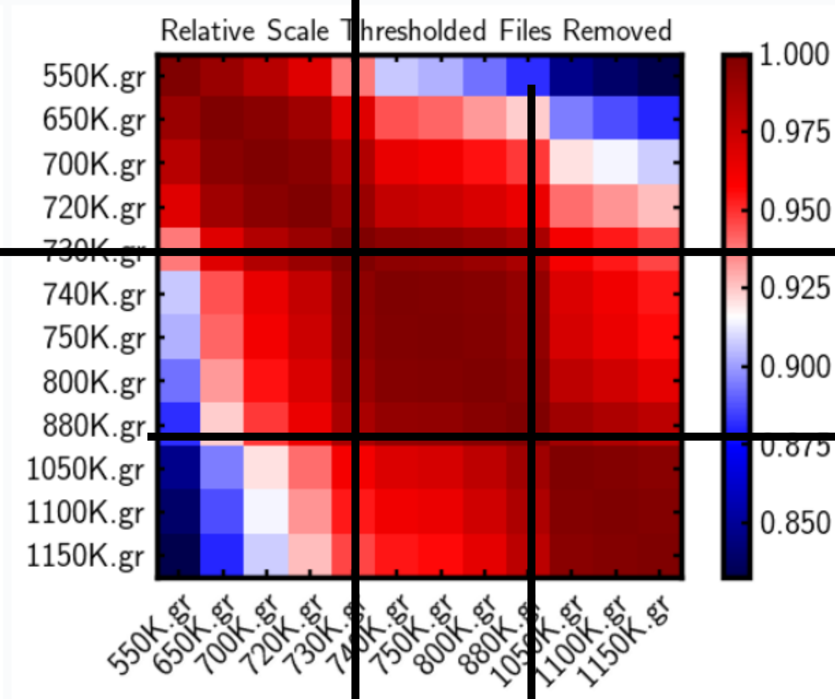

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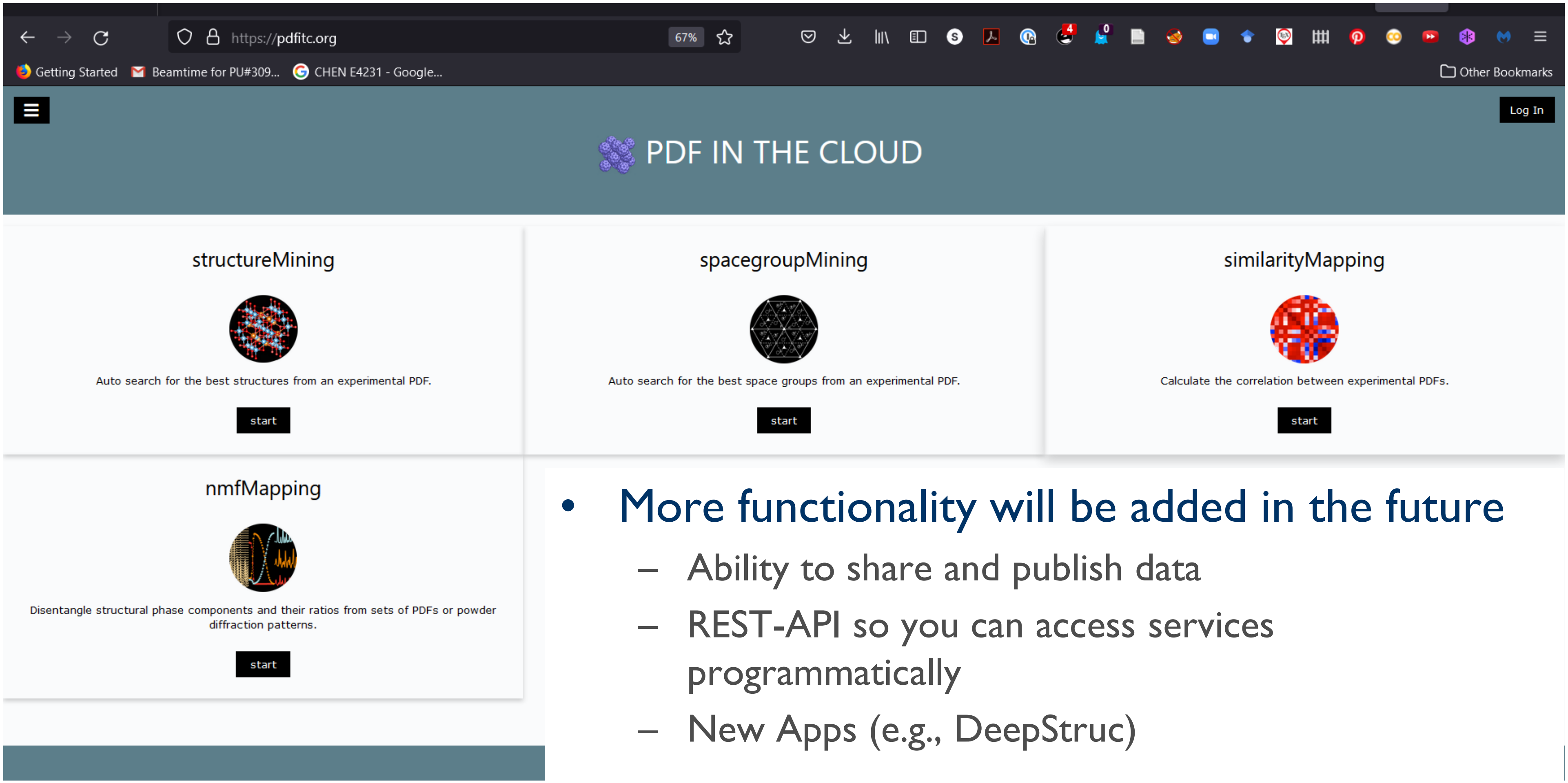

- More functionality will be added in the future
  - Ability to share and publish data
  - REST-API so you can access services programmatically
  - New Apps (e.g., DeepStruc)
  - …

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Summary

- PDF continues to grow in popularity
  - More and more materials of interest are nanostructured or amorphous

- PDF continues to become more powerful with faster measurements
  - In situ, spatially resolved etc.

- ePDF is set to become widely used because of its ease and ability to study very small volumes, and ease of doing spatially resolved at the nanometer lengthscale

- This raises issues with data handling and modeling. These are being addressed with high throughput analysis and modeling methods

Acknowledgements

- A special thank you to all my current and former students and post-docs
- Facility beamline and software teams
- Also my many wonderful collaborators, mentioned during the talk
- Facilities:
  - APS, CHESS, NSLSII (and people therein)
  - MLNSC, ISIS, SNS (and people therein)
- Funding: DOE-BES and NSF-DMR

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Science in the Zoom times