

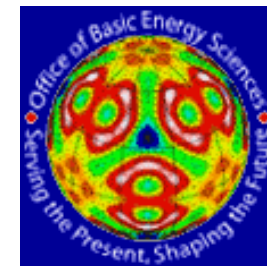
# Complex Modeling: towards more robust nanostructure refinements

**S.J.L. Billinge**

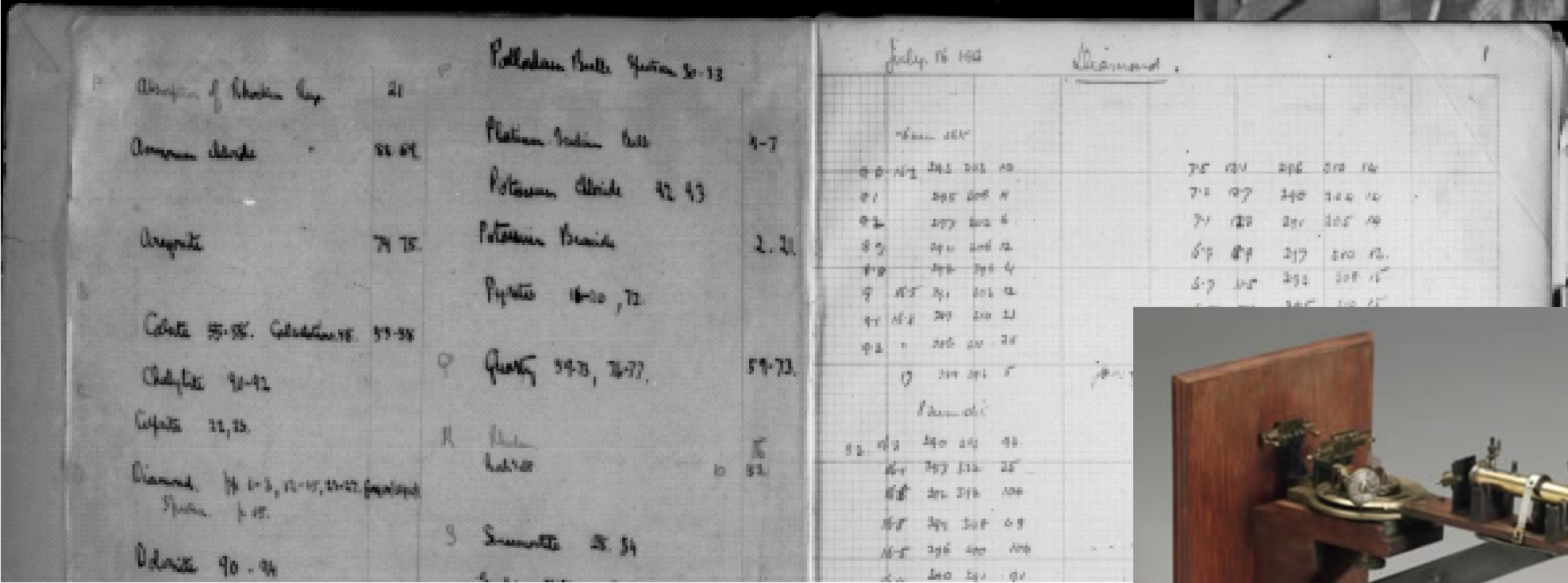
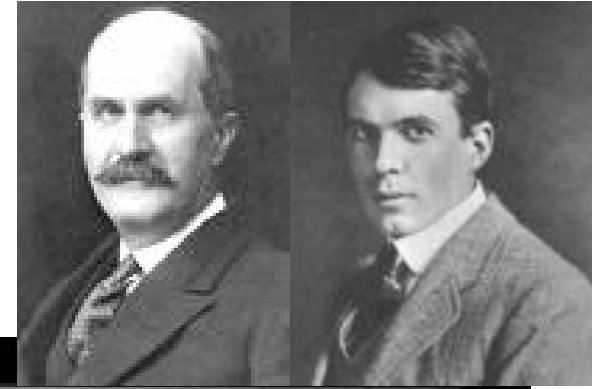
*Department of Applied Physics and Applied Mathematics*

*Columbia University,*

*CMPMS, Brookhaven National Laboratory*



# W. Henry Bragg's notebook

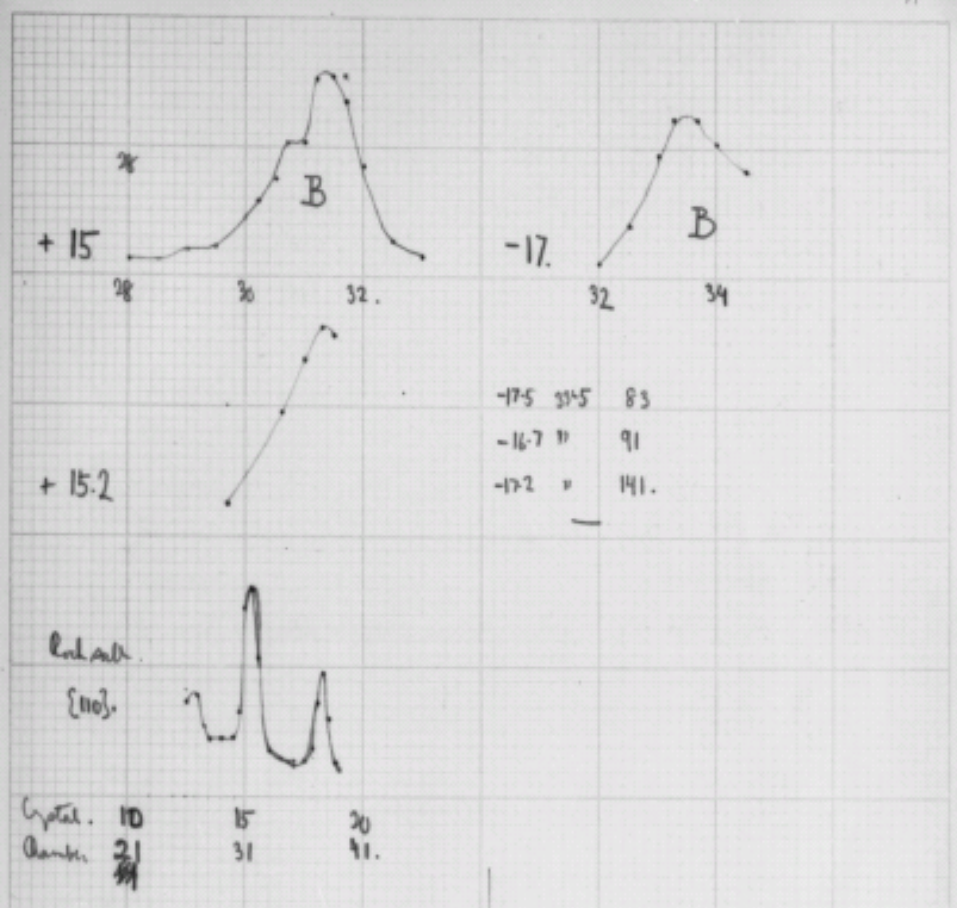


• Available at U. Leeds website:  
<http://www.leeds.ac.uk/library/spcoll/bragg-notebook/>

[110] Rock Salt. large bits. 10 sec.  
Readings taken on paper as 11th book was not available.

Angles. +26.7°	+31.3	+37.4	$\sin 2\theta = .2710$
-(28.9)	-33.5	-(39.6)	$\sin 11.6 = .2011$
			Ratio 1.34.
Means 27.8	32.4	38.5	
15.9	16.2	19.2.	

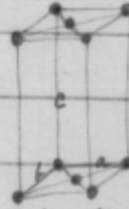
When taking these readings the bulb was blue nearly all over, the anticathode spot being very large and a blue line stretching from cathode to anticathode.  
Quartz gave absolutely no reflection, apparently.



- Page 11, he has moved from diamond to rock-salt...the first appearance of something looking like a Bragg peak

(consider the 'block')  
 imagine a face centred lattice axes, edges a, b, c. and that 16 atoms  
 of sulphur are in each block.

$$S.G. = 2.07$$



$$\text{Vol of block} = 16 \times 32 \times 164 \times 10^{-24} = 838 \times 10^{-24}$$

$$\text{Vol of block} = \frac{838 \times 10^{-24}}{2.07} = 405 \times 10^{-24}$$

$$\therefore abc = 1.545 \times 10^3 = 405 \times 10^{-24}$$

$$b^3 = 262 \times 10^{-24}$$

$$b = 6.4 \times 10^{-8}$$

$$a = .812, a^3 = .661, \frac{1}{a} = 1.513$$

$$c = 1.803, c^3 = 5.832, \frac{1}{c} = .276$$

$$\text{Hence } I^r \text{ from } 000 \text{ on } 111 \text{ plane} = \frac{1}{\sqrt{\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}}} = \frac{b}{\sqrt{2.789}} = \frac{b}{1.67} = .5928 \times b = 3.83$$

$$000 \text{ on } 011 = \frac{1}{2\sqrt{\frac{1}{b^2} + \frac{1}{c^2}}} = \frac{b}{2\sqrt{1.276}} = \frac{b}{2.26} = .4425 \times b = 2.83$$

$$000 \text{ on } 001 = \frac{1}{1.405 \cdot b} = 1.405 \cdot b = 12.18$$

$$P_1 = .577 \times 10^{-8} \quad 000 \text{ on } 010 = .6 \cdot b = .500 \cdot b = 3.20$$

$$000 \text{ on } 100 = .913 \cdot b = .406 \cdot b = 2.60$$

Hence reflections should occur at the following angles. (b, law  $\sin \theta = \frac{\lambda}{2d}$ )

(111) (011) (001) (010) 100 (110) (101)

$\frac{\lambda}{2d}$  .0754 .1019 .0233 .0902 .1109 .071 .119.

Calc.  $\theta$  4.3° 5.85° 1.33° 5.2° 6.35° 4.1° 6.02°

Exp.  $\theta$  4.75° 5.90° 10.5° (10.8°) 5.15° 6.2° 4.07° 7.0° p.45

$$I^r \text{ on } 110 = \frac{1}{\sqrt{\frac{1}{a^2} + \frac{1}{b^2}}} = \frac{b}{\sqrt{2.073}} = .635 \times b = 4.06 \cdot b$$

$$I^r \text{ on } 101 = \frac{1}{2\sqrt{\frac{1}{a^2} + \frac{1}{b^2}}} = \frac{b}{2\sqrt{2.073}} = .756 \times b = 4.84 \cdot b$$

$$\sin 1.33 = .0233$$

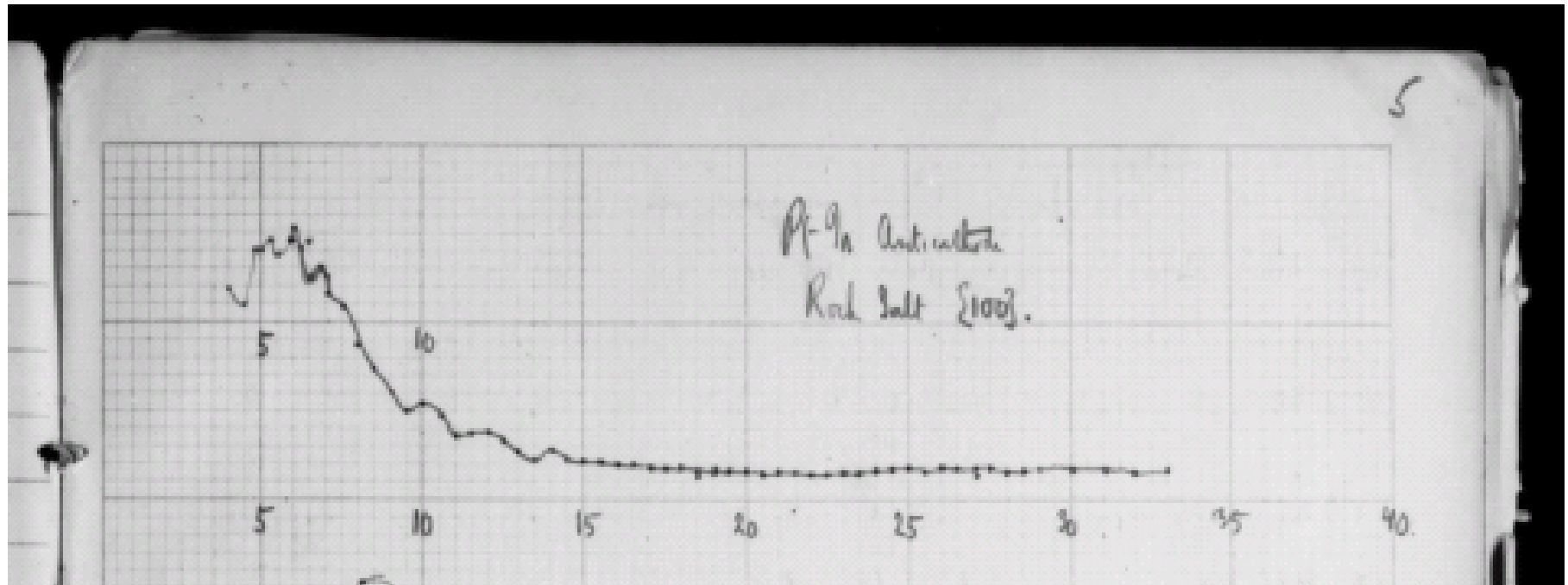
$$\sin 10.65 = .1849$$

$$\frac{10.19}{8} = .1274$$

- Apparently the first structure solution
- Page 43

# Diffuse Scattering

- The Braggs discovered Bragg scattering on Page 11
- But apparently they discovered diffuse scattering on Page 5!

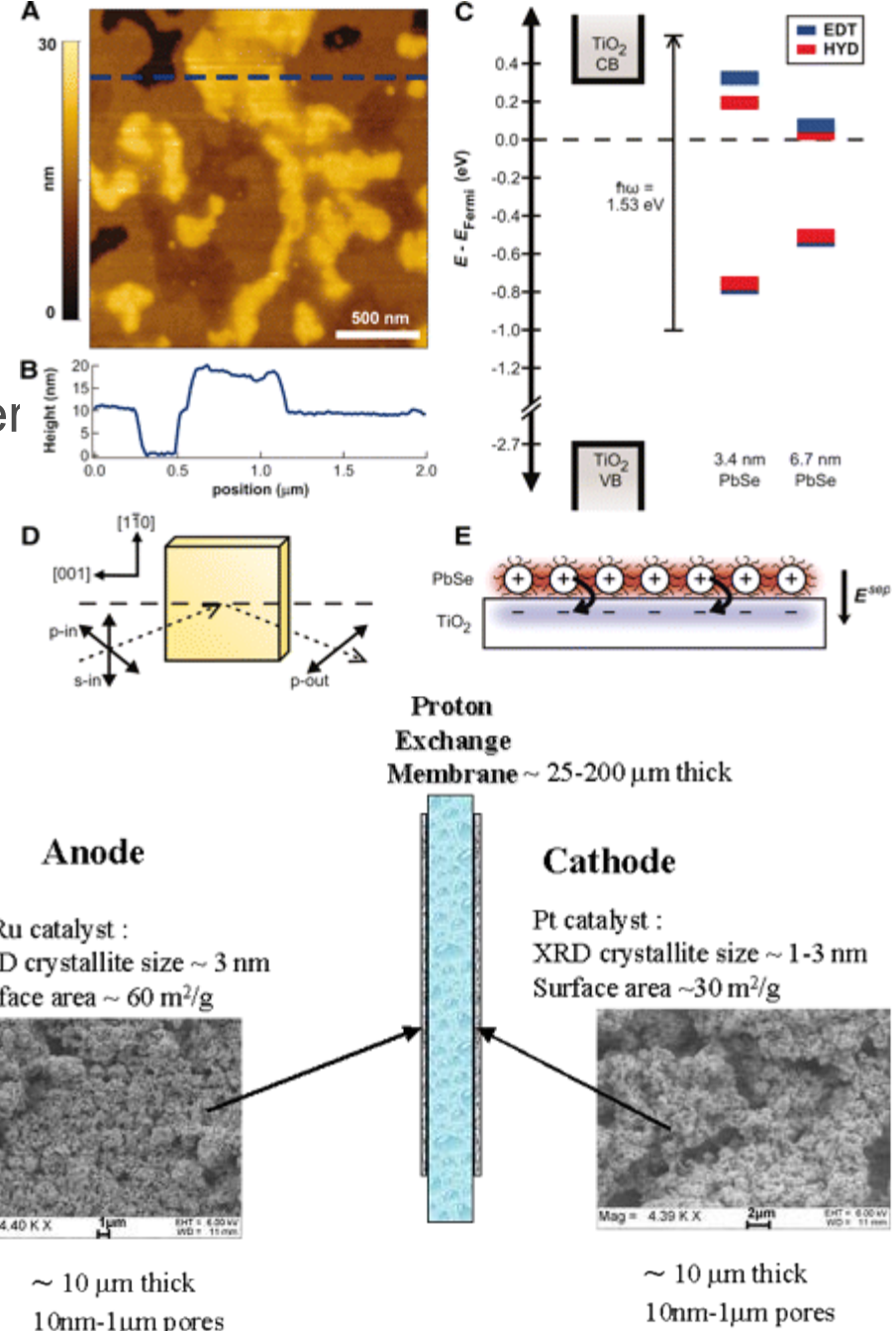


# Overview of talk

1. Scientific need: to understand complex materials for next generation technologies
2. Scientific problem: they are complex!
3. Example: the nanostructure problem
4. Generic solution
5. Summary and outlook

# Complex materials

- Photovoltaics with improved efficiency
  - Nanoparticles in the light collecting layer
- High energy density batteries
  - Electrodes
  - Electrolytes
- Fuel cells for transportation applications
  - Electrodes
  - Electrolytes
  - Catalysts
  - Hydrogen storage
- Sequestration
  - Functionalized mesoporous materials



# Recurring themes in Complex Materials:

They have

- Structure at the nanoscale
  - E.g., just about everything
- Complicated structures, large unit cells, multiple elements
  - E.g., thermoelectrics, next generation battery materials, etc..
- Sub-micron heterogeneities
  - E.g., core-shell nanoparticles, supported catalysts, real devices

**Enormous experimental and theoretical challenges in Complex Materials**



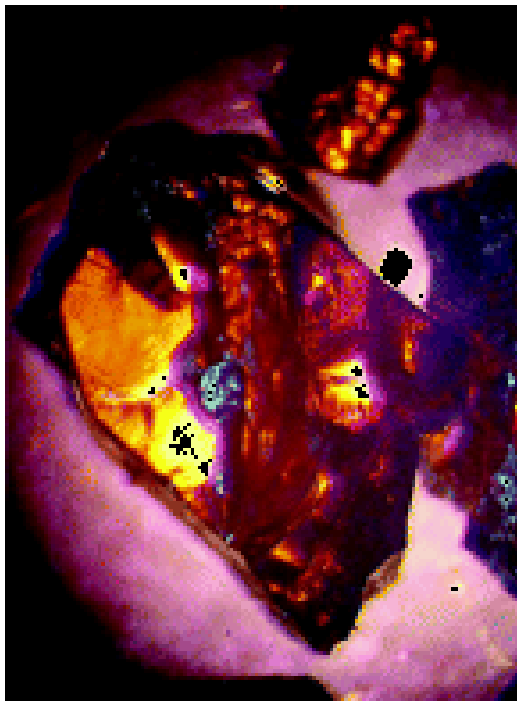
# The Complexity Problem

To solve today's technological problems we need to study materials systems at the frontier of complexity.

An example of the complexity problem:

The nanostructure problem

# The Crystal Structure Problem

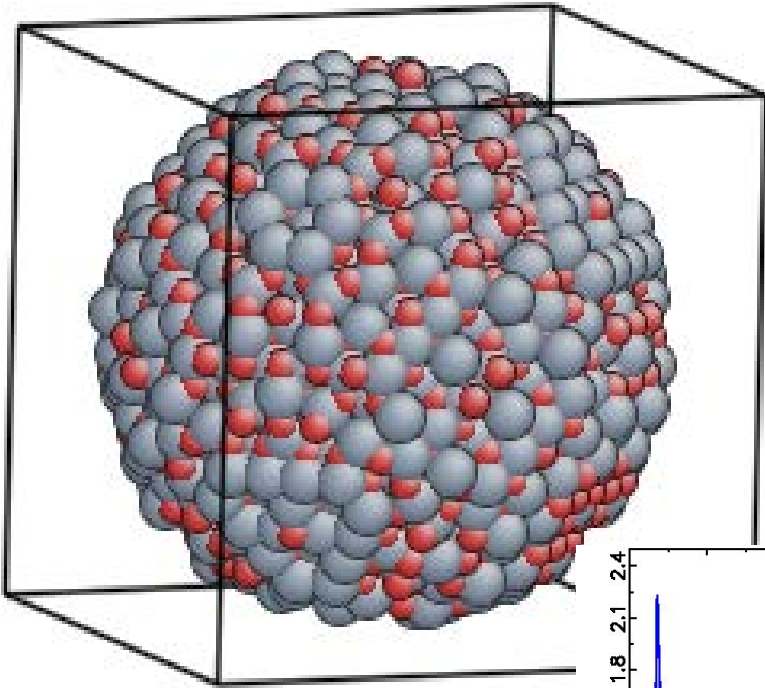


- Problem:
  - Here is a crystal, what is its structure?
- Solution:
  1. Give it to your grad student
  2. She puts it on the x-ray machine
  3. ...Pushes the button
    1. Machine tells you the structure
    2. Or Machine gets stuck
      1. Throw away the crystal
      2. Make it the subject of her thesis

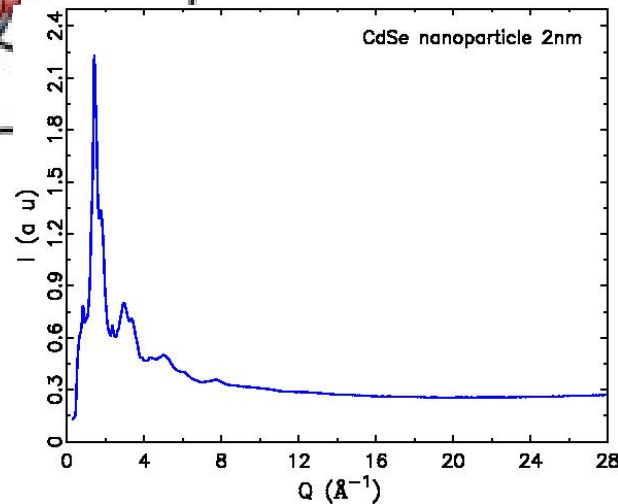
Crystallography is largely a solved problem

From LiGaTe<sub>2</sub>: A New Highly Nonlinear  
Chalcopyrite Optical Crystal for the Mid-IR  
L. Isaenko, et al., J. Crystal Growth, 5, 1325  
– 1329 (2005)

# The Nanostructure Problem



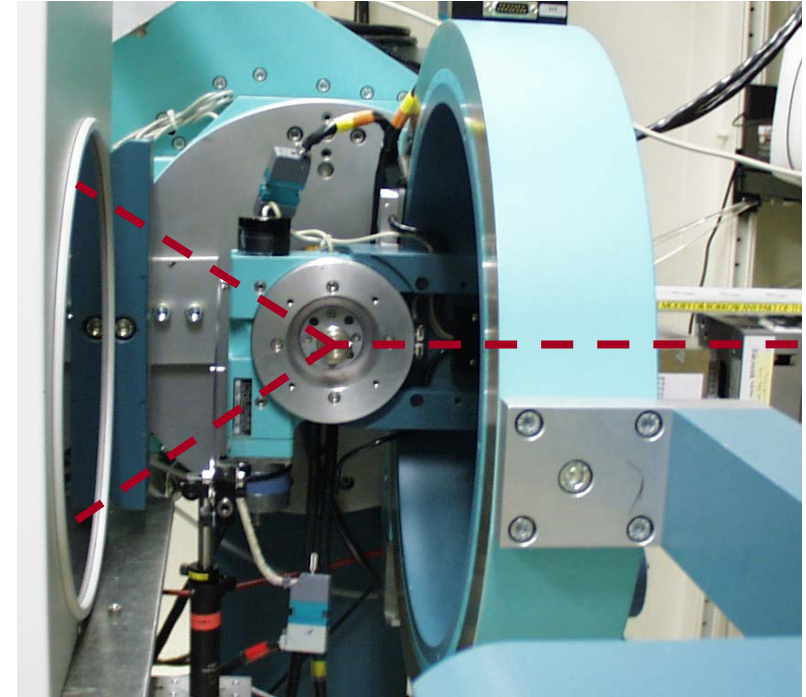
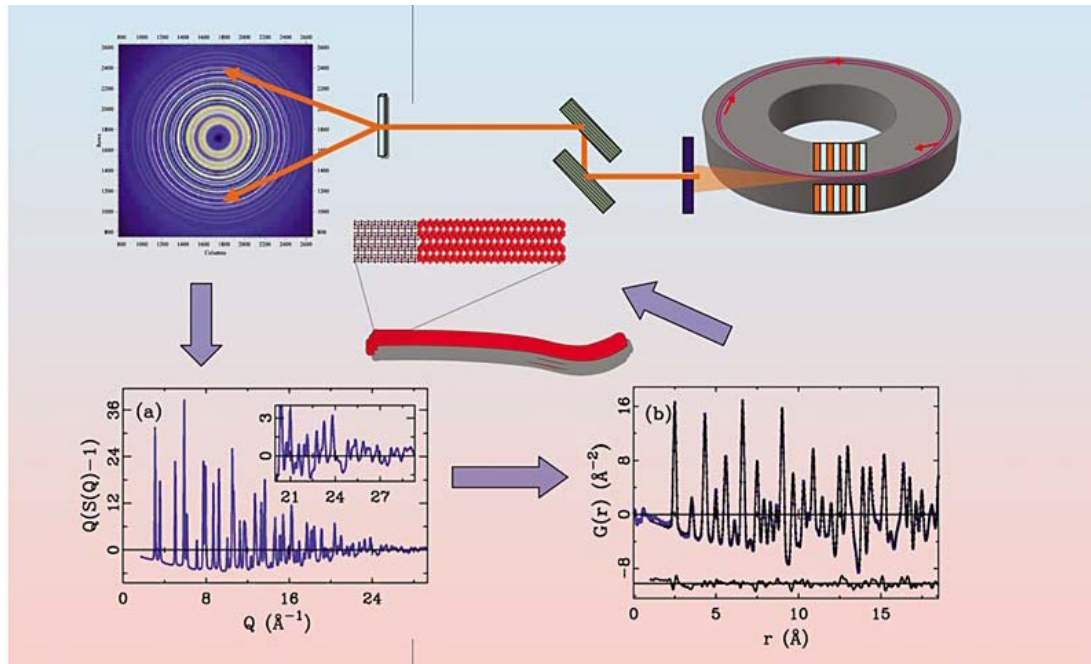
- **Problem:**
  - Here is a nanoparticle, what is its structure?
- **Solution:**
  1. Give it to your grad student
  2. She puts it on the x-ray machine
  3. ...Pushes the button



# X-ray PDF Experiment

RAPDF – Rapid Acquisition PDF

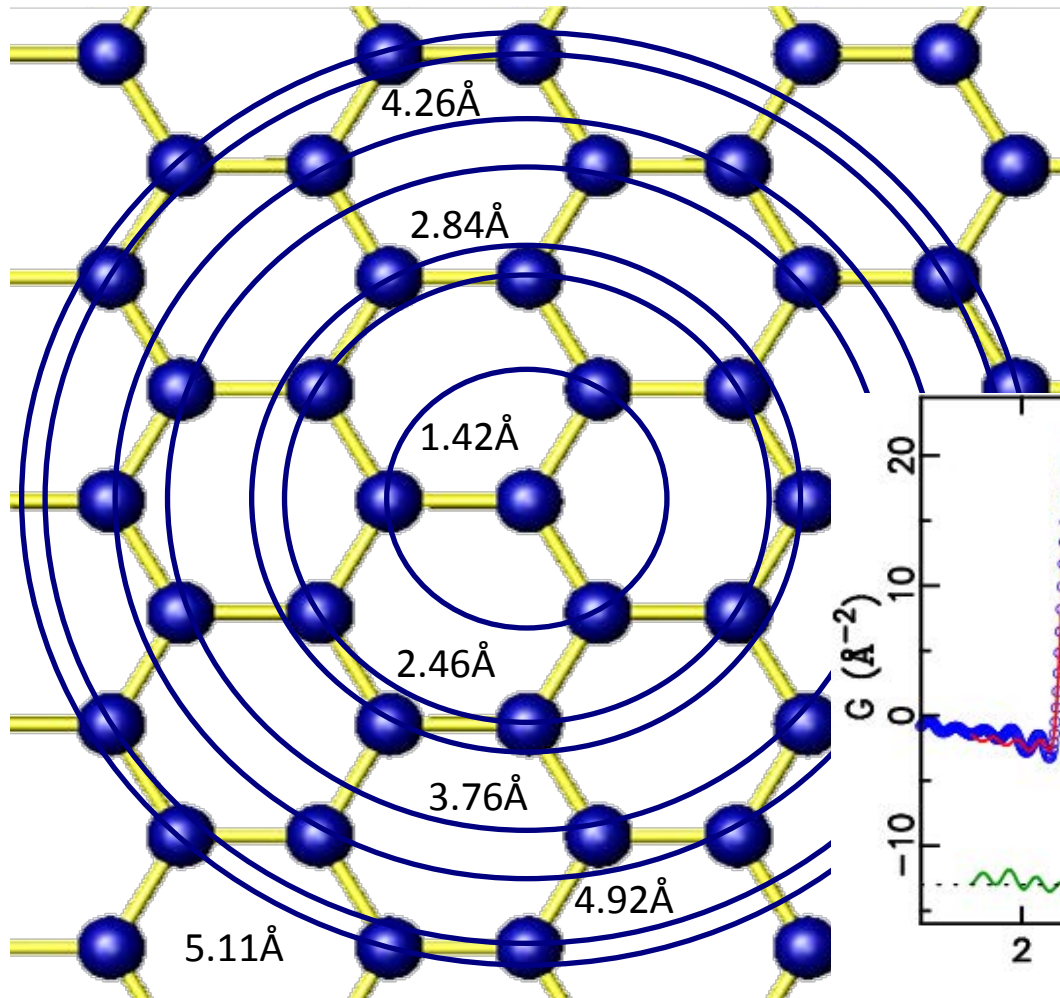
- few second measurement time



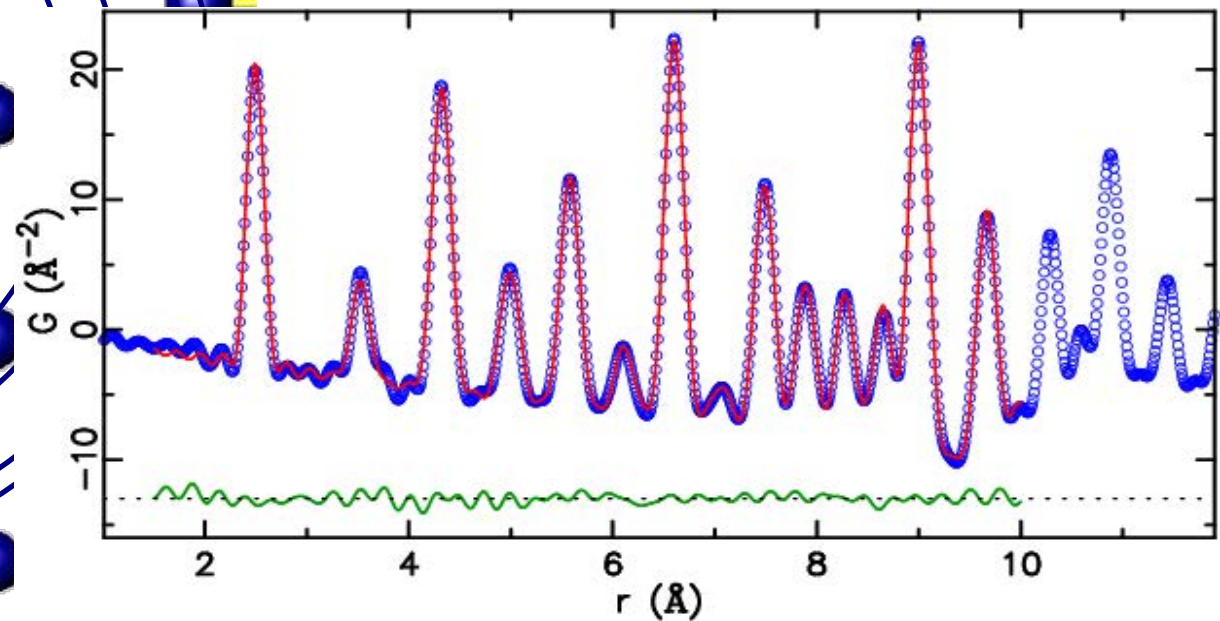
- Chupas et al., J. Appl. Crystallogr. (2003)
- Billinge-group, BNL, SUNY-SB, APS collaboration
- Main developments thanks to Pete Chupas and Xiangyun Qiu



# Nanostructure refinement



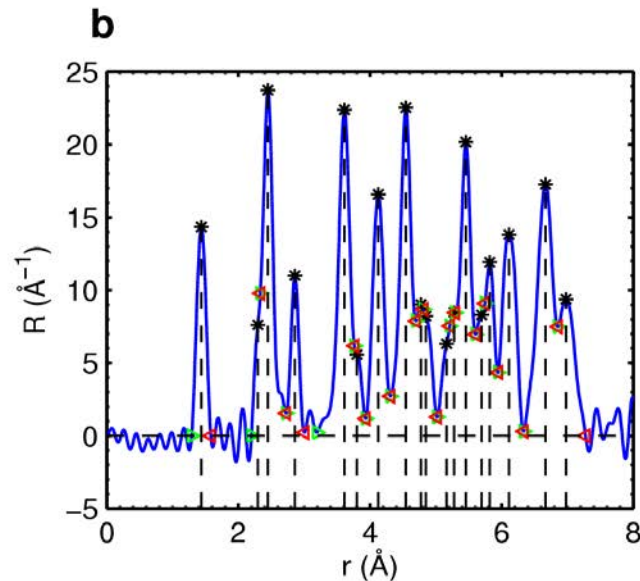
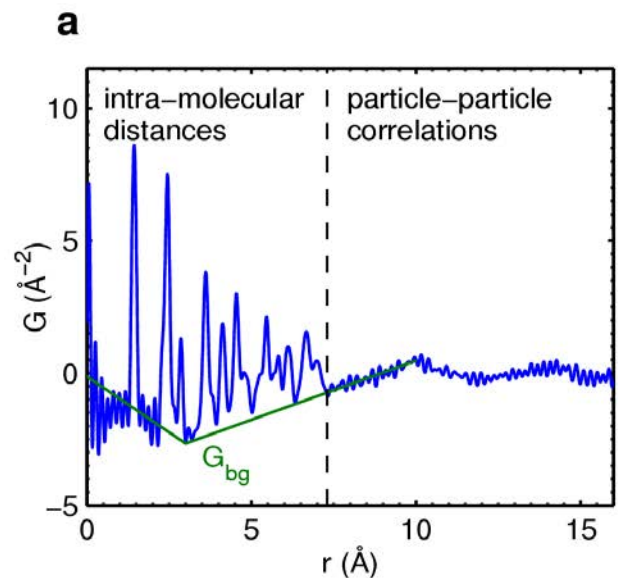
Pair distribution function (PDF) gives the probability of finding an atom at a distance “r” from a given atom.



# Structure Solution from PDF

## Example: C60

- 60 atoms  $\Rightarrow n(n-1)/2 = 1770$  pair-vectors
- We know the lengths (not the directions) of  $\sim 18$  unique distances
- We have an imperfect measure of the multiplicities of those distances
- We don't have any symmetry information to help us



Is the problem well conditioned or ill conditioned?  
Is there a unique solution?

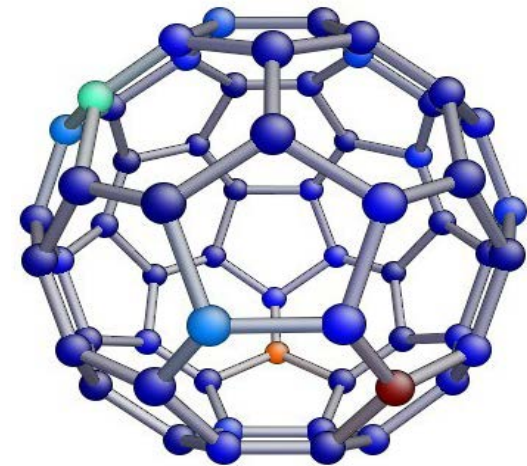
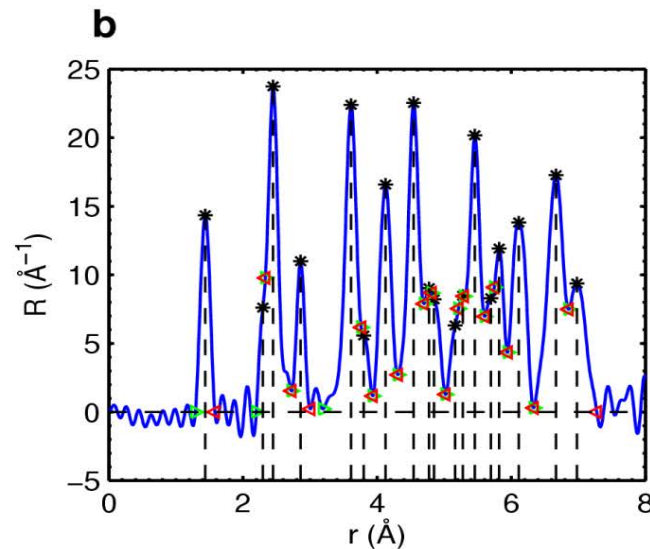
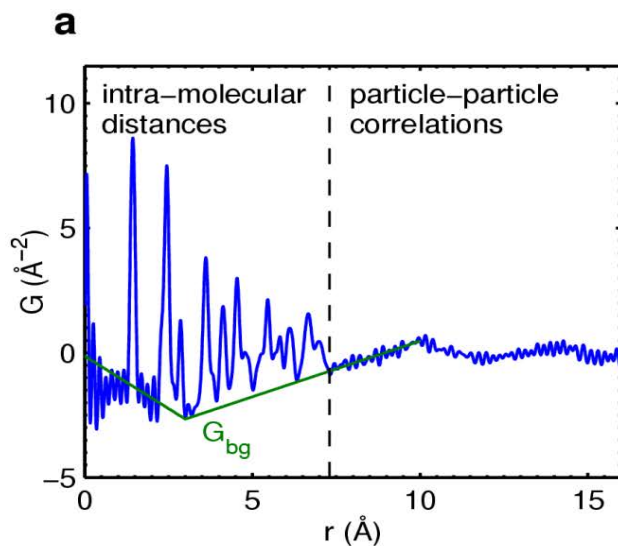
# Structure Solution






# Structure determination from PDF

- neutron diffraction PDF data from  $C_{60}$
- 60 atoms, 1770 distances
- extracted 18 out of 21 unique distance values
- structure determination still successful



low error  high error

[Juhás et. al, Nature 440, 655-658 (2006)]

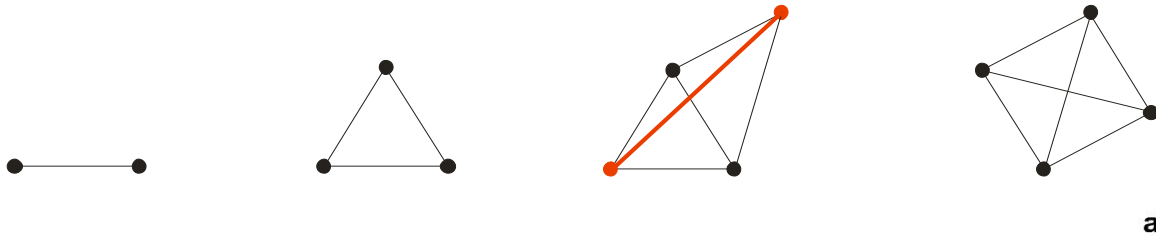
[Juhás et. al, Acta Cryst. A 64, 631-640 (2008)]

- algorithm extended for multiple atom-types and periodic boundary conditions



# Illustration of cluster buildup

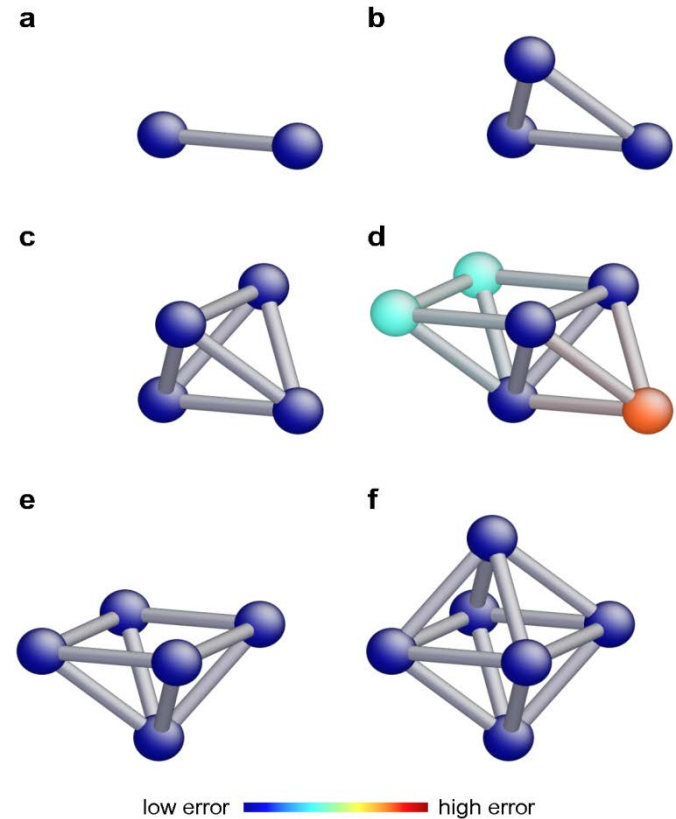
- square-distances =  $[4 \times 1, 2 \times \sqrt{2}]$



- octahedron-distances =  $[12 \times 1, 3 \times \sqrt{2}]$

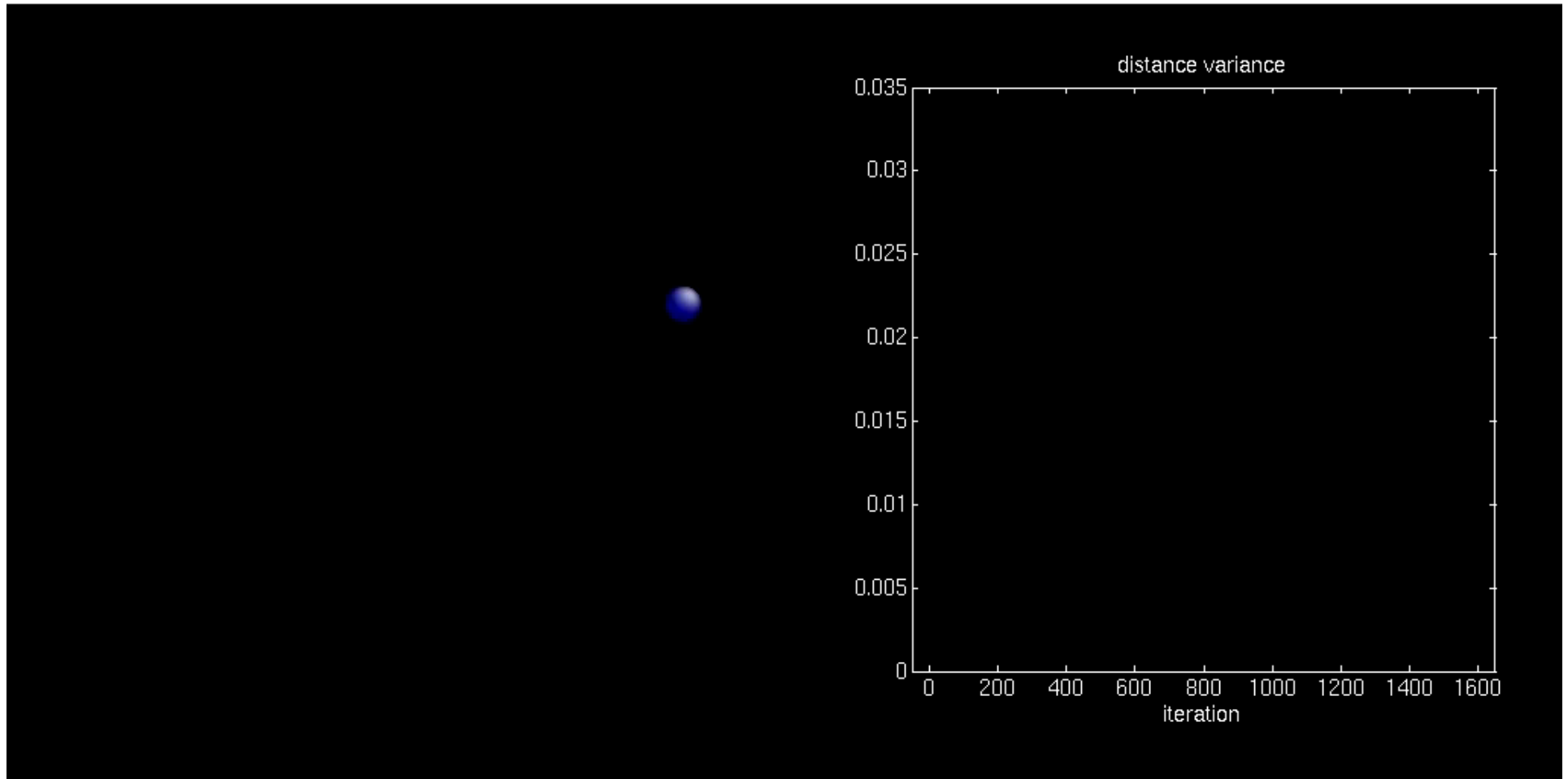
- minimized cost function:

$$\text{var}(d) = \frac{1}{P} \sum_{k=1}^P [d_k - t_{l(k)}]^2$$

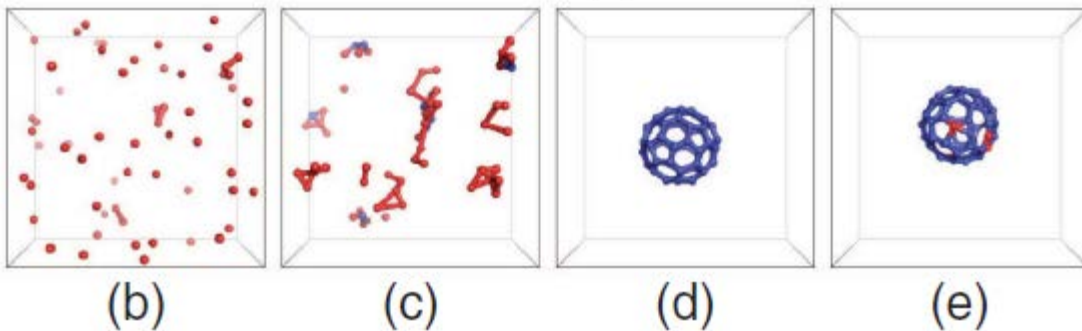
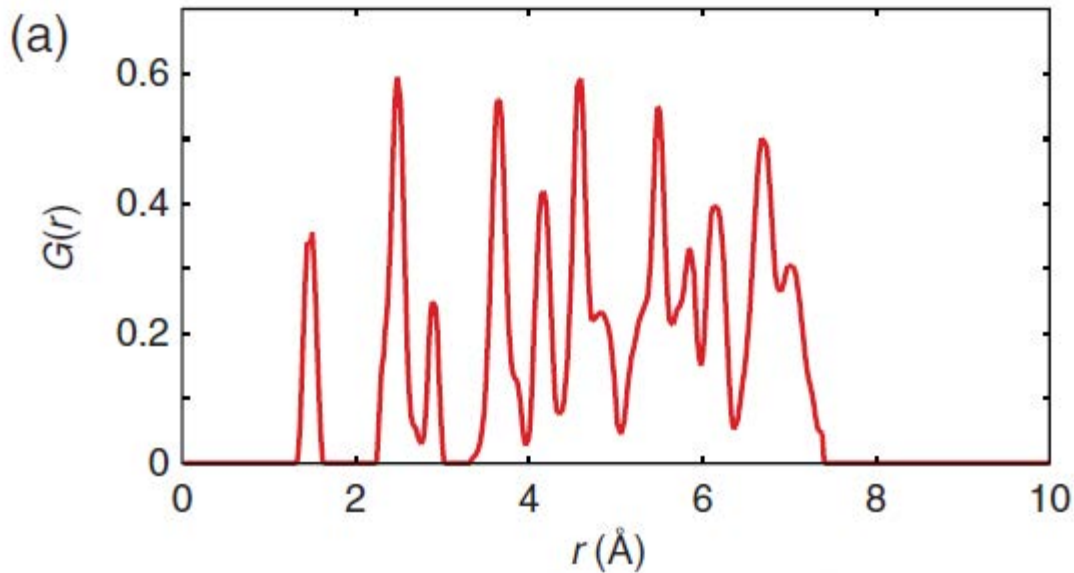


Juhas, SJB et al., Nature 2006

# *ab-initio* structure solution directly from PDF data



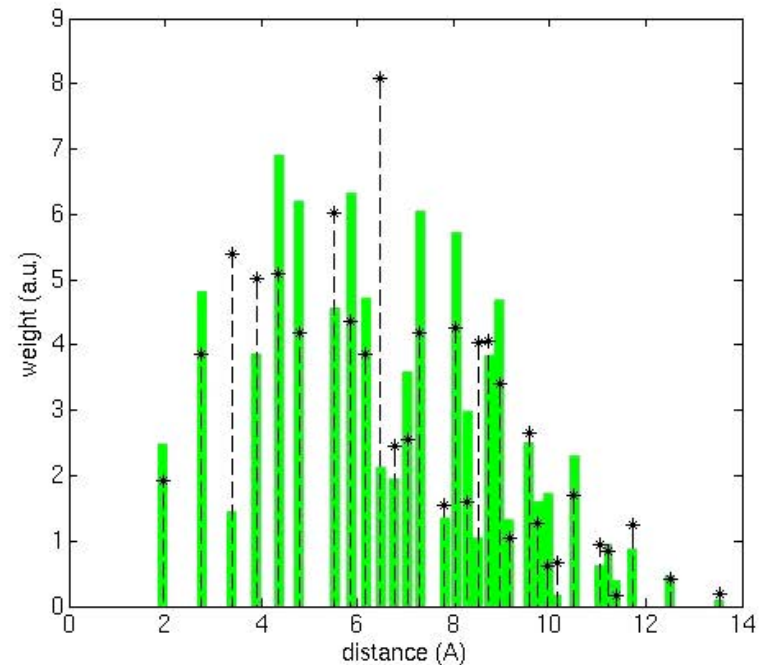
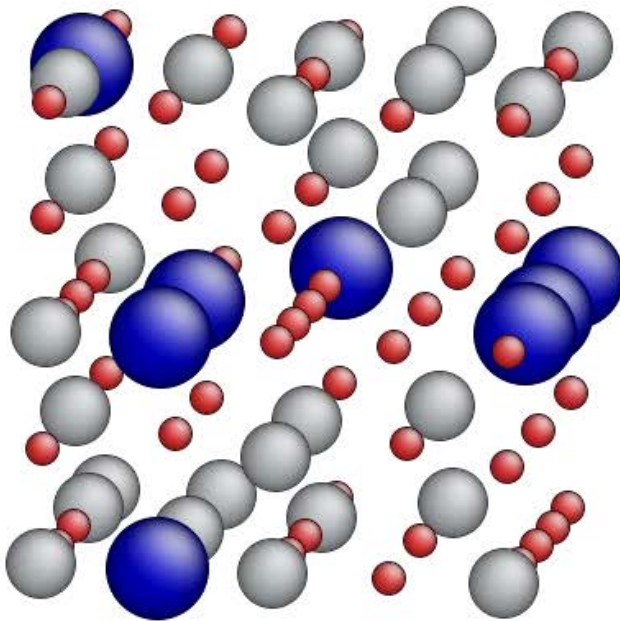
# C60 structure from RMC + similarity constraint



- Simulated annealing could solve the C60 problem only with the addition of an extra “similarity” constraint (all carbon atoms have the same environment).
- This example shows that adding constraints not only regularizes inverse problems but also can increase efficiency of regression algorithms.
- Cliffe, Andrew L. Goodwin et al. **Structure determination of disordered materials from diffraction data**, *Phys. Rev. Lett.* **104**, 125501 (2010).

# Multi-element structure solutions from the PDF

- Crystal structure solution from the PDF
  - start with random site arrangement
  - flip sites which improve match between model and ideal peak weights



# Crystal structure solution from experimentally determined atomic pair distribution functions

P. Juhás,<sup>a\*</sup> L. Granlund,<sup>b</sup> S. R. Gujarathi,<sup>b</sup> P. M. Duxbury<sup>b</sup> and S. J. L. Billinge<sup>a,c</sup>

<sup>a</sup>Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA, <sup>b</sup>Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA, and <sup>c</sup>Condensed Matter Physics and Materials Science Department, Brookhaven

Journal of  
Applied  
Crystallography

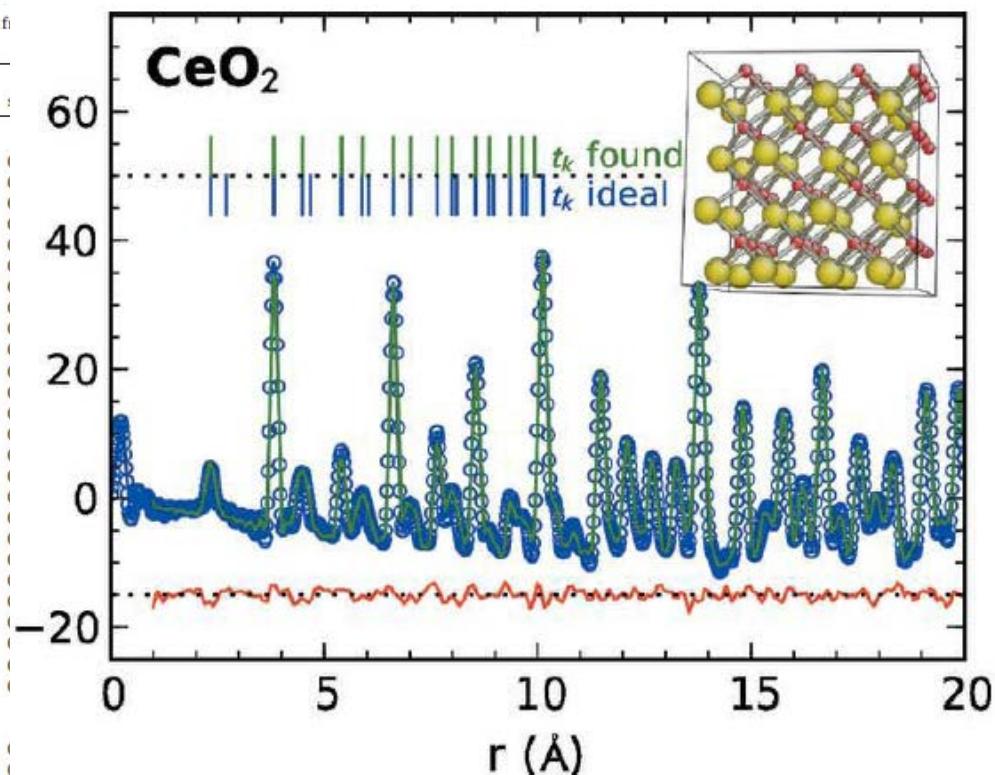
ISSN 0021-8898

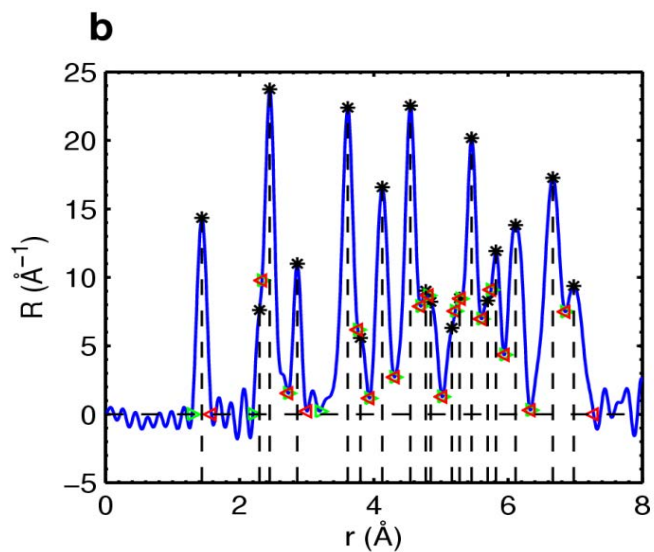
Received 20 October 2009

Accepted 16 March 2010

$C_d$  and  $C_c$  are the distance and atom-overlap costs, as defined in equations (3) and (4).  $s_x$ ,  $s_y$  and  $s_z$  are the standard deviations in the  $r$  normalized to a simple [111] cell.  $s_r$  ( $\text{\AA}$ ) is the root mean-square displacement of the solved sites from the reference CIF positions.

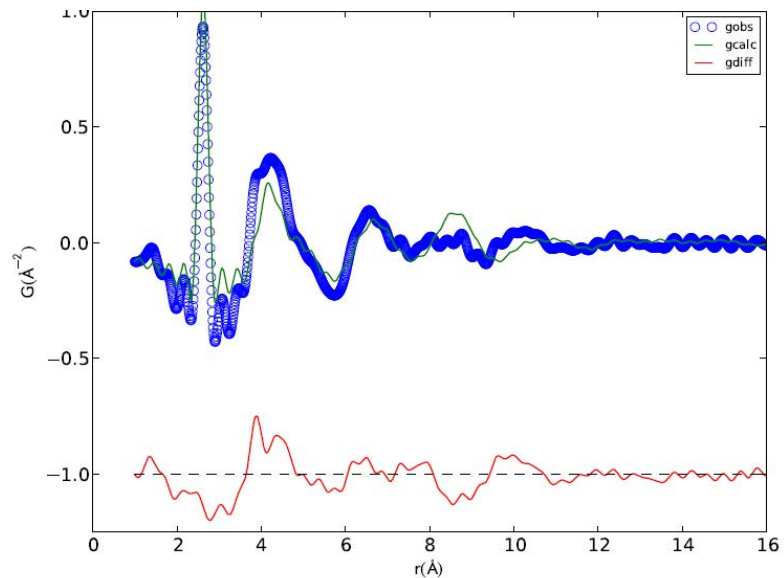
Sample (supercell)	Atoms	Cost $C_d$ ( $0.01 \text{\AA}^2$ )		Cost $C_c$ ( $\text{\AA}^2$ )		Deviation of coordinates	
		Liga	CIF	Liga	CIF	$s_x$	$s_y$
<b>Successful solutions</b>							
Ag [111]	4	0.0232	0.136	0	0.001	0	0
Ag [222]	32	0.0097	0.136	0	0.001	0.00025	0.00024
BaTiO <sub>3</sub> [111]	5	0.370	0.394	0.040	0.042	0.0057	0.0066
BaTiO <sub>3</sub> [112]	10	0.392	0.394	0.058	0.042	0.00023	0.039
C graphite [111]	4	0.396	0.574	0.010	0.016	0.0029	0.0029
C graphite [221]	16	0.420	0.574	0.010	0.016	0.0086	0.0065
CdSe [111]	4	0.107	0.138	0	0.001	0	0
CdSe [221]	16	0.0856	0.138	0	0.001	0.00010	0.00013
CeO <sub>2</sub> [111]	12	0.515	0.554	0	0	0	0
NaCl [111]	8	1.75	1.71	0	0	0	0
NaCl [222]	64	1.20	1.71	0	0	0.00031	0.00031
Ni [111]	4	0.0024	0.0024	0	0	0	0
Ni [222]	32	0.0025	0.0024	0	0	0.00015	0.00013
PbS [111]	8	0.0125	0.0104	0.010	0.011	0	0
PbS [222]	64	0.0140	0.0104	0.010	0.011	0.00005	0.00004
PbTe [111]	8	0.0024	0.0127	0.097	0.090	0	0
PbTe [222]	64	0.0022	0.0127	0.097	0.090	0.00011	0.00011
Si [111]	8	0.0045	0.0045	0	0	0	0
Si [222]	64	0.0048	0.0045	0	0	0.00010	0.00009
SrTiO <sub>3</sub> [111]	5	0.437	0.437	0.002	0.002	0	0
Zn [111]	2	0.495	0.470	0	0	0	0
Zn [222]	16	0.564	0.470	0	0	0.00010	0.00006
ZnS sphalerite [111]	8	0.150	0.0647	0	0	0	0
ZnS sphalerite [222]	64	0.160	0.0647	0	0	0.00029	0.00033
ZnS wurtzite [111]	4	0.141	0.152	0	0	0	0
ZnS wurtzite [221]	16	0.165	0.152	0	0	0.00003	0.00002
<b>Failed solutions</b>							
CaTiO <sub>3</sub> [111]	20	0.4967	0.902	0.52	0.072	0.16	0.14
TiO <sub>2</sub> rutile [111]	6	0.5358	0.758	0.40	0.009	0.081	0.24





60 atoms

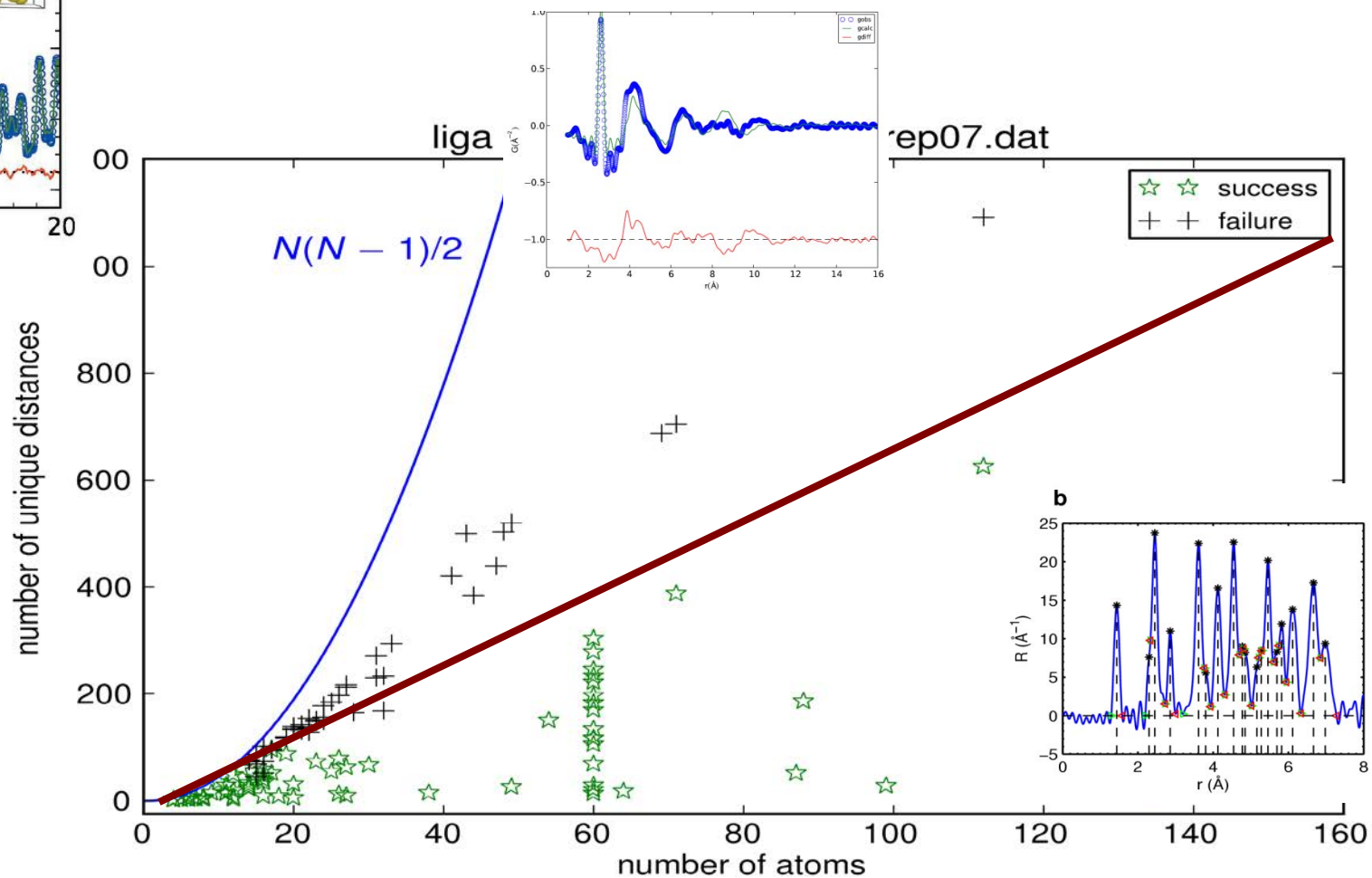
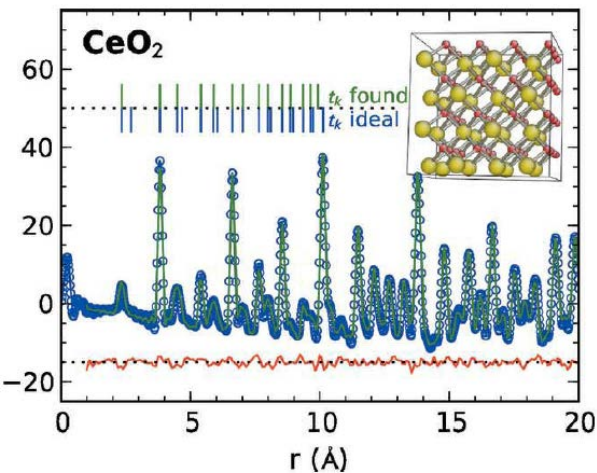
$C_{60}$



~64 atoms

Ultra-small CdSe NPs

# Successology





# Problem

Well posed problem:

Information in the PDF data

Degrees of freedom in the model

# Problem

As the complexity of the structural solution increases:

Information in the PDF data

Degrees of freedom in the model

# Problem

Solution is ill-posed:

Degrees of freedom in the model

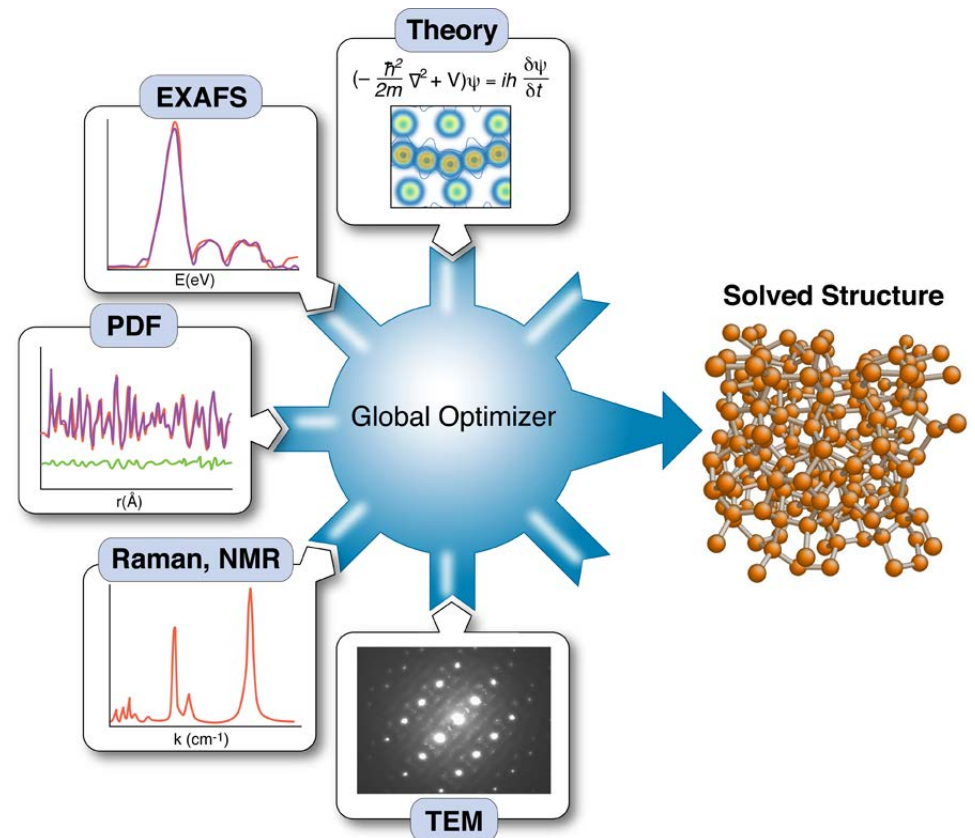
Information in the PDF data

# Structure Solution



# Complex Modeling

- $c = a + ib$  – complex number mixes real and imaginary parts
- $m = e + it$  – complex modeling mixes experiment and theory in a coherent computational framework
- Billinge and Levin, Science 2007



# Complex modeling (CM) is a continuous spectrum

- Rietveld refinement of two datasets or two banks of neutron data is (local search) CM
- Rietveld refinement + rigid body constraints is (local search) CM
- Parametric refinement is (local search) CM
- RMC refinement including diffraction profiles and  $G(r)$  is (local search) CM
- RMC + similarity constraints on C60 is (global search) CM

**We seek more robustness and more flexibility**

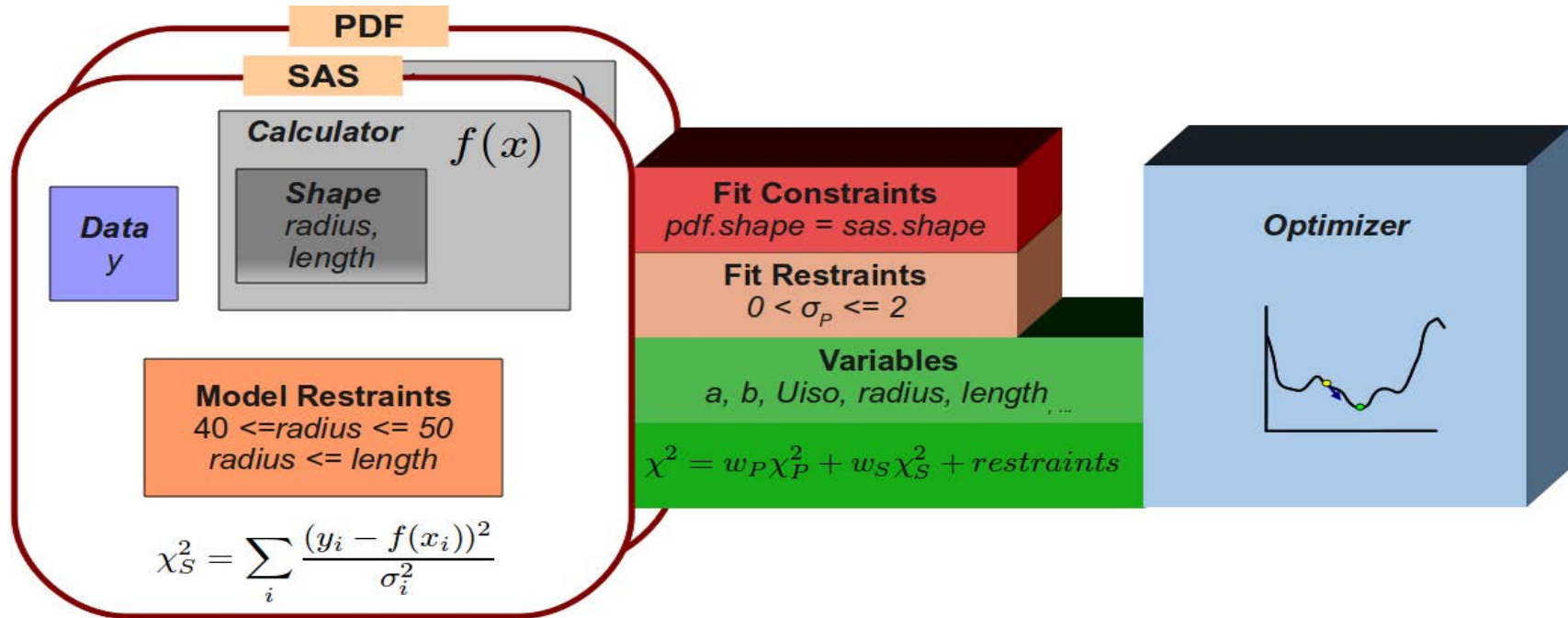
Life After PDFgui:

SrFit and SrReal

Modular and Extensible

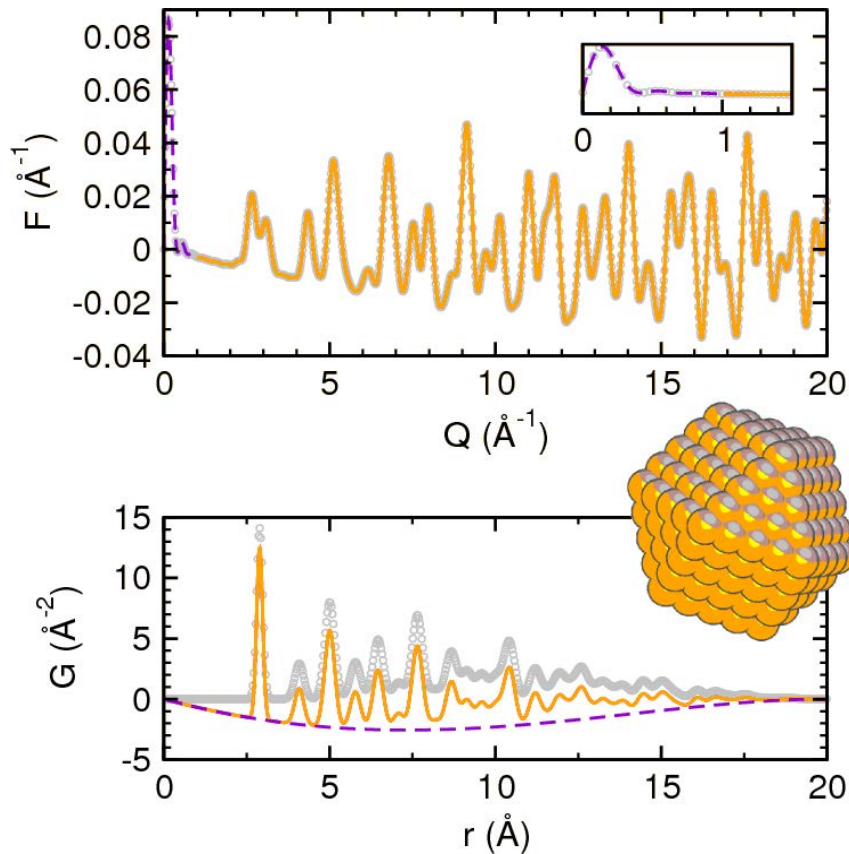
# Complex Modeling – SrFit – Modular!

- Python framework for Complex Modeling
  - Build a cost function from available forward calculators and data
  - Each “page” a separate cost function
  - Pages tied together with common variables and a unified cost function
- Interfaces with existing software
  - DANSE diffraction for PDF
  - DANSE SANS for SAS
- Developed by Chris Farrow and Pavol Juhas



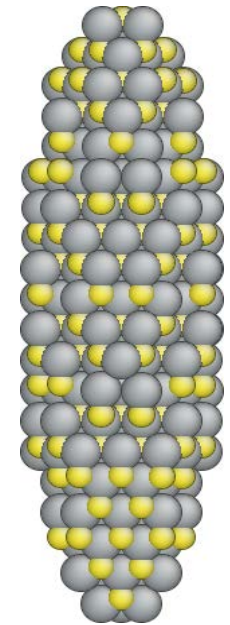
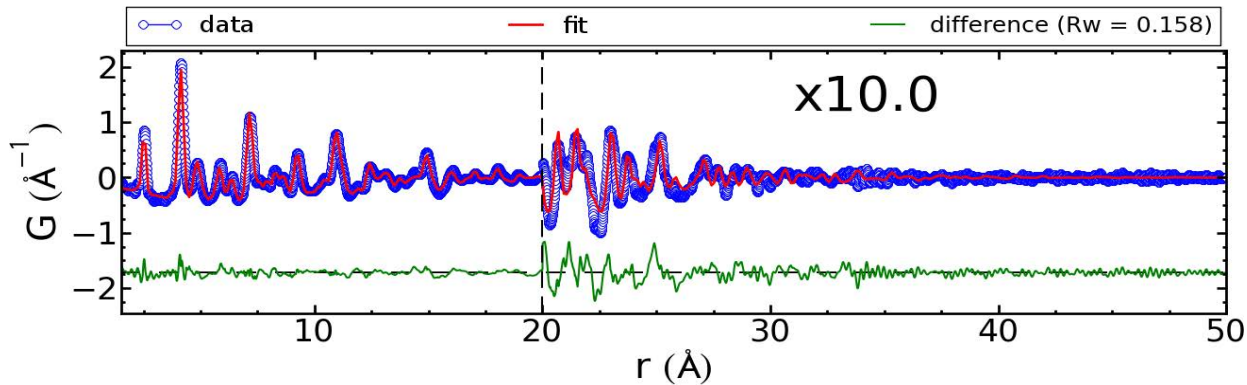


# Bottom line: including SAS data yields a different correlation function: $R(r)$ vs. $G(r)$



- SAS usually not measured
- “shape transform” captured in diffraction peaks
- Without SAS, average density subtracted out
- With SAS: the background of the  $G(r)$  function is obtained

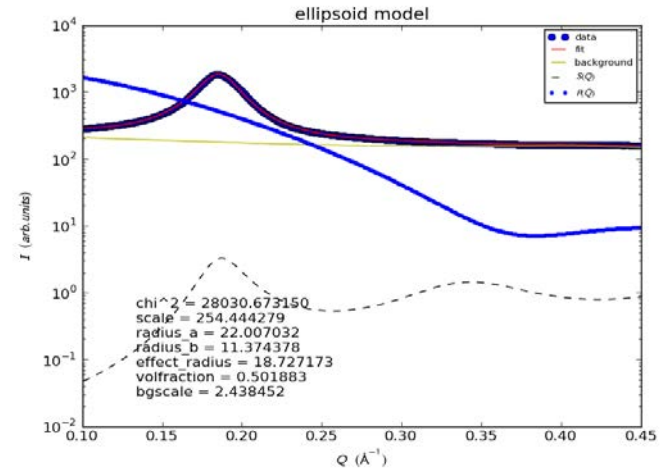
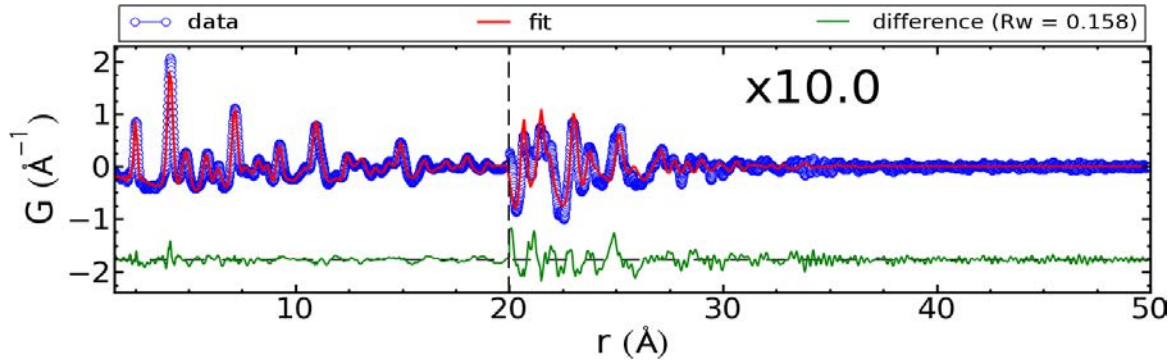
# PDF



.Modeled as spheroidal nanocrystals with approximate stacking fault model, homogeneous strain effects

- .Model refines with  $\sim 3.5:1$  aspect ratio
- .Approximately 25% stacking fault density
- .Shape parameters correlated with peak width (thermal) parameters
- .Model does not capture inhomogeneous strain in the first two peaks

# PDF + SAXS Complex



.PDF and SAS shape parameters tied together, combined residual

TABLE I. Structural and shape parameters from CdS nanoparticles determined by PDF and SAXS using a spheroidal model. Results for the wurtzite phase are shown below (Cd at  $(1/3, 2/3, 0)$ , S at  $(1/3, 2/3, z)$ ).

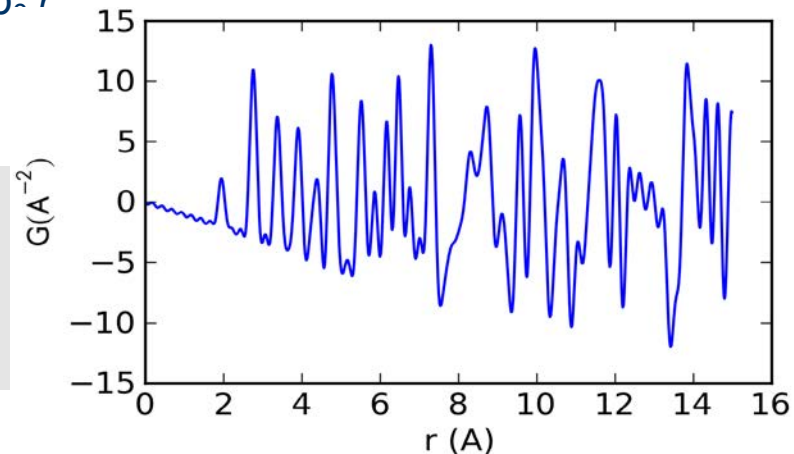
	SAXS	PDF	Complex
$R_w$ (PDF)	-	0.146	0.155
$R_w$ (SAXS)	0.0148	-	0.0150
$a$ ( $\text{\AA}$ )	-	4.134	4.134
$c$ ( $\text{\AA}$ )	-	6.753	6.761
S Z-frac.	-	0.441	0.418
Cd $U_{iso}$ ( $\text{\AA}^2$ )	-	0.0936	0.0098
S $U_{iso}$ ( $\text{\AA}^2$ )	-	0.0158	0.0166
wurtzite fraction	-	0.355	0.402
equatorial radius ( $\text{\AA}$ )	11.36	10.17	11.37
polar radius ( $\text{\AA}$ )	20.77	32.43	21.80

# SrFit - ExtensiblePDFCalculator

- PDF calculation in real-space
  - suitable for periodic systems
  - one structure per calculator → mixed-phase PDFs obtained by combining several PDFCalculator objects
- other results: radial distribution function, partial PDFs,  $F(Q)$
- class ScatteringFactorTable
  - lookup of xray, neutron or electron scattering factors
  - support for custom scattering factors
- class PeakProfile – the profile function for a pair contribution
- class PeakWidthModel – calculates profile width for a given atom pair
- class PDFEnvelope – one or more r-dependent scaling envelopes
- class PDFBaseline – the baseline function, by default  $-4\pi\rho \cdot r$

## example:

```
>>> from diffpy.Structure import Structure
>>> from diffpy.srreal.pdfcalculator import PDFCalculator
>>> sto = Structure(filename='SrTiO3.cif')
>>> pdfc = PDFCalculator(rmax=15, qmax=25)
>>> r, g = pdfc(sto)
>>> import pylab
>>> pylab.plot(r, g)
```



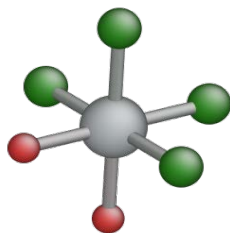
# DebyePDFCalculator

- PDF calculation in Q-space –  $F(Q)$  calculated by Debye scattering equation and Fourier transformed to  $G(r)$

$$F(Q) = \frac{1}{N \langle f(Q) \rangle^2} \sum_{i,j} f_i(Q) f_j(Q) \frac{\sin Q r_{ij}}{r_{ij}} \exp \left[ -\frac{1}{2} \sigma_{ij}^2 Q^2 \right]$$

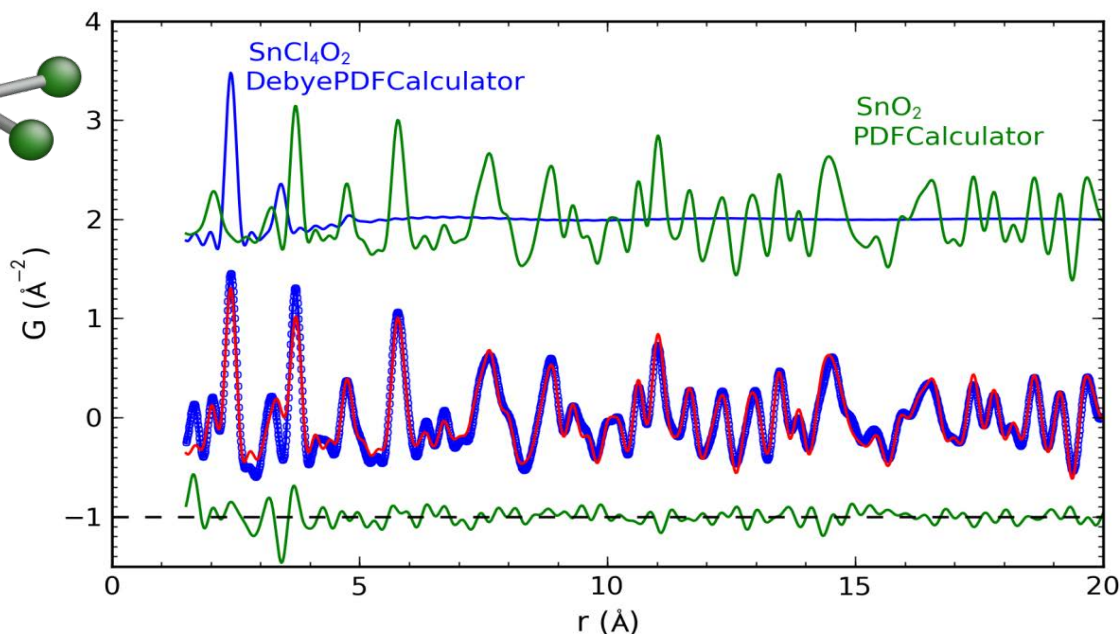
$$G(r) = \frac{2}{\pi} \int_{Q_{\min}}^{Q_{\max}} F(Q) \sin Q r \, dQ$$

- suitable for molecules or nano-clusters
- PDF baseline simulated by  $Q_{\min}$  cutoff in the calculated  $S(Q)$



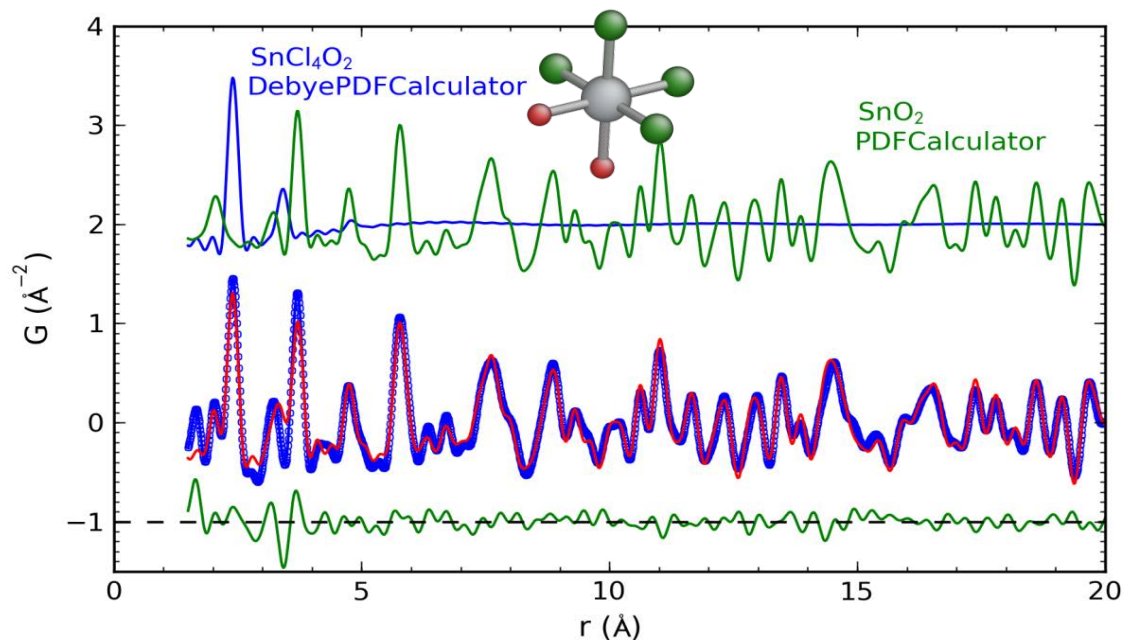
example:

- work by Kirsten L. Jensen, Aarhus Universitat, Denmark
- in-situ studies of  $\text{SnO}_2$  formation from  $\text{SnCl}_4 \cdot 5\text{H}_2\text{O}$
- time dependence of the precursor – target ratios

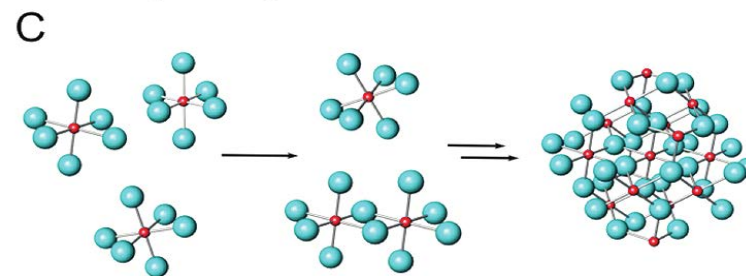
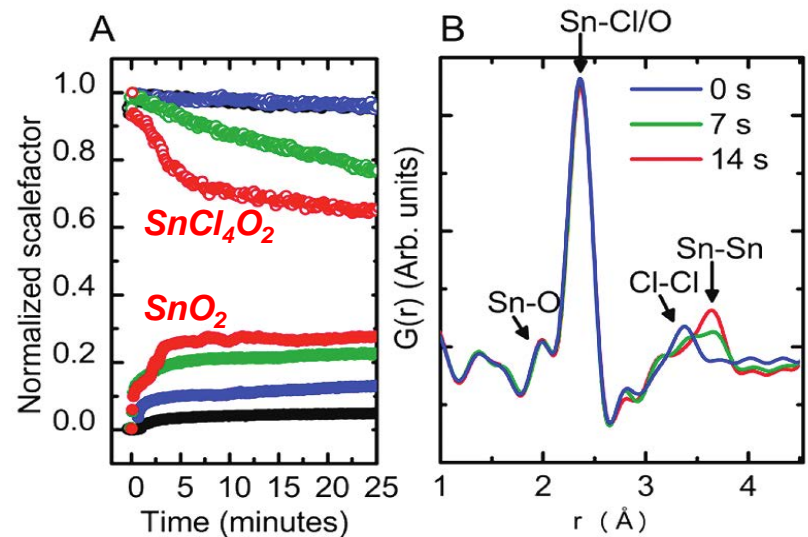


# PDF analysis of in situ SnO<sub>2</sub> formation

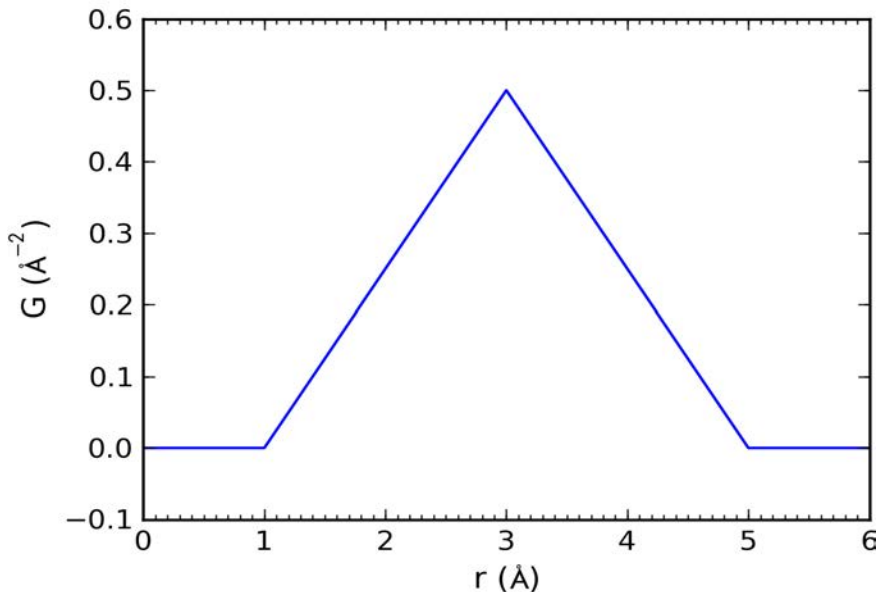
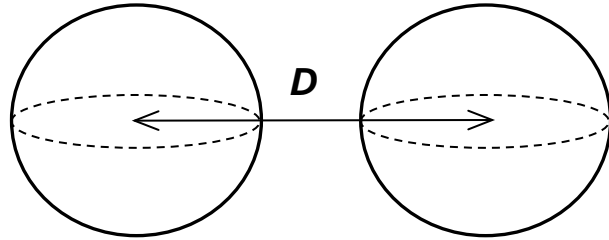
- in-situ studies of SnO<sub>2</sub> formation during hydrothermal synthesis,
- PDF measured every 7 seconds at an synchrotron x-ray source
- measured PDFs were fitted as a two-phase mixture of SnCl<sub>4</sub>·2H<sub>2</sub>O molecules and SnO<sub>2</sub> crystallites
- time dependence of the precursor-target ratios and the crystallite size



K. M. Jensen, et al., J. Am. Chem. Soc., 134, 6785 (2012)



# SrFit – Extensible!



- PDF from two spherical shells can be calculated analytically

$$G(r) = \frac{1}{S_1 S_2 r} \iint_{S_1 S_2} \delta(r - r_{12}) dS_1 dS_2$$

triangular profile centered at spheres' distance D

- cluster of spherical shells → PDF calculation requires triangular profile function
- non-standard PDF profile requires
  - definition of a new profile function
  - telling PDFCalculator to use the new profile

# Custom PDF peak profile

profile defined in C++

```
#include <cmath>
#include <diffpy/srreal/PeakProfile.hpp>

using diffpy::srreal::PeakProfile;
using diffpy::srreal::PeakProfilePtr;

class SphericalShellsProfile : public PeakProfile {
public:
    PeakProfilePtr create() const {
        return PeakProfilePtr(new SphericalShellsProfile());
    }

    PeakProfilePtr clone() const {
        return PeakProfilePtr(new SphericalShellsProfile(*this));
    }

    const std::string& type() const {
        static std::string tp = "spherical shells-cpp";
        return tp;
    }

    double yvalue(double x, double fwhm) const {
        if (fabs(x) > fwhm) return 0.0;
        double rv = (fwhm - fabs(x)) / (1.0 * fwhm * fwhm);
        return rv;
    }

    double xboundlo(double fwhm) const { return -fwhm; }
    double xboundhi(double fwhm) const { return +fwhm; }
};

bool reg_SawToothProfile = SphericalShellsProfile().registerThisType();
```

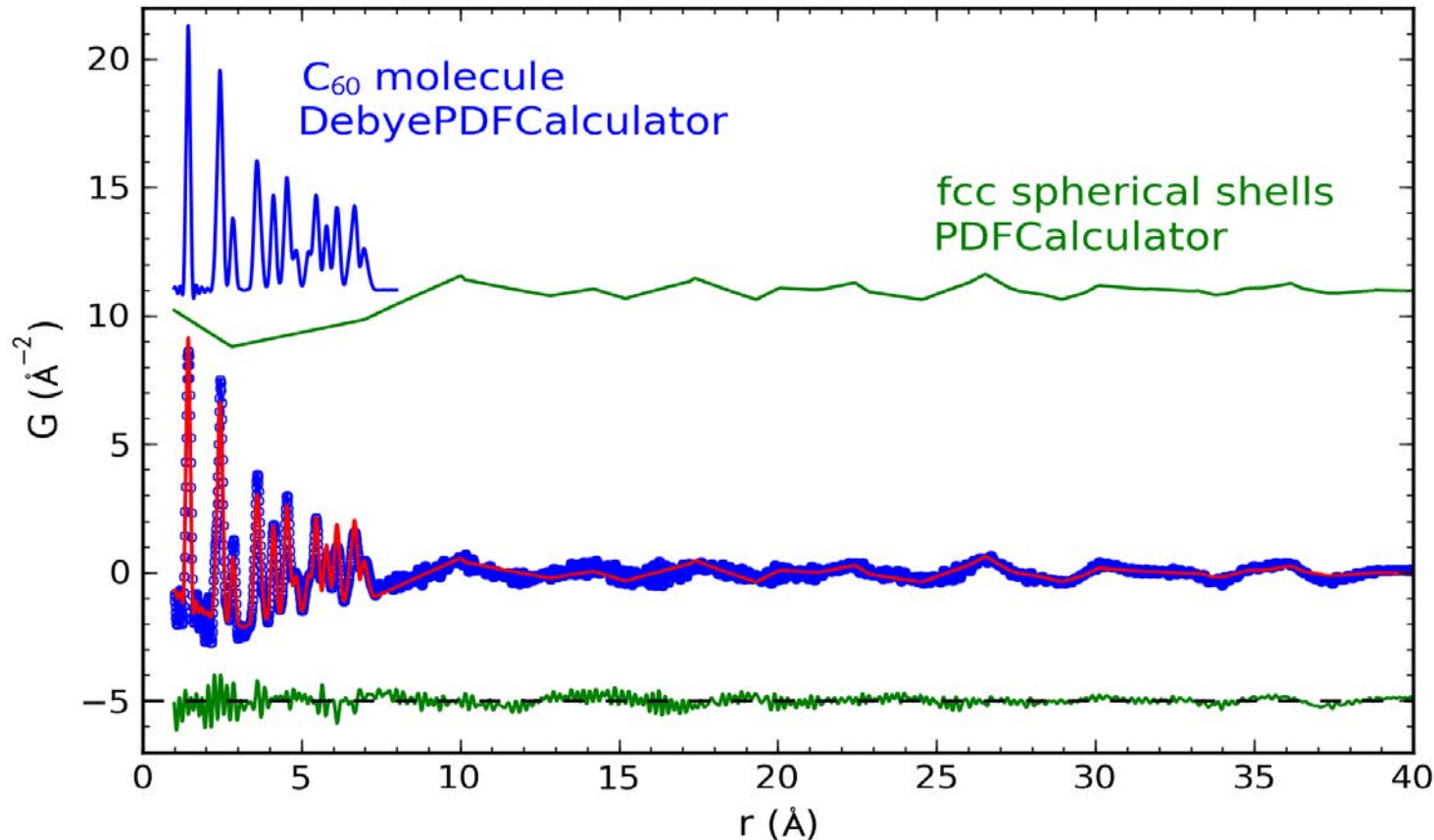
profile used in Python

```
>>> from diffpy.srreal.pdfcalculator import PeakProfile, PDFCalculator
>>> PeakProfile.getRegisteredTypes()
set(['croppedgaussian', 'gaussian'])
>>> import ctypes
>>> ctypes.cdll.LoadLibrary('./sphericalshells-cpp.so')
>>> PeakProfile.getRegisteredTypes()
set(['sphericalshells-cpp', 'croppedgaussian', 'gaussian'])
>>> pdfcalc = PDFCalculator()
>>> pdfcalc.setPeakProfileByType('sphericalshells-cpp')
```

- new profile functions can be defined either in Python or C++
- for C++ the profile function is compiled as a dynamic link library sphericalshells-cpp.so
- on loading the library adds new profile to the global registry → profile ready for use in Python
- no need to rebuild any other C++ sources related to PDFCalculator
- no need to write any Python wrappers for the new profile function



# PDF refinement of fcc C<sub>60</sub>



fit residuum  $R_w = 0.26$

scale ratio = 60.0(1)

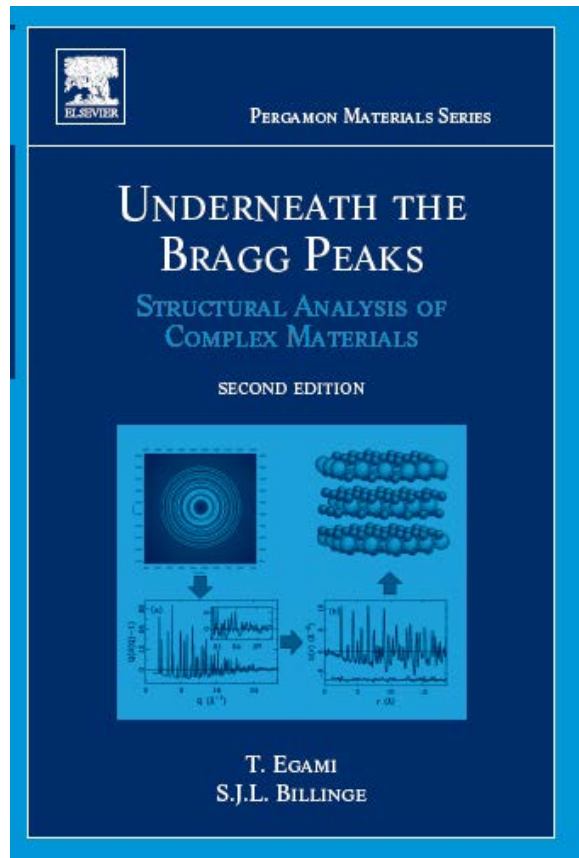
$U_{iso} = 0.00323(4)$

molecule diameter = 7.113(2)    shell diameter = 7.22(4)

- PDF from fcc C<sub>60</sub> can be refined on the full measured range accounting for both intra and inter-molecular correlations

# Data reduction to get the PDF

- Traditional Approach, apply all the physical corrections:

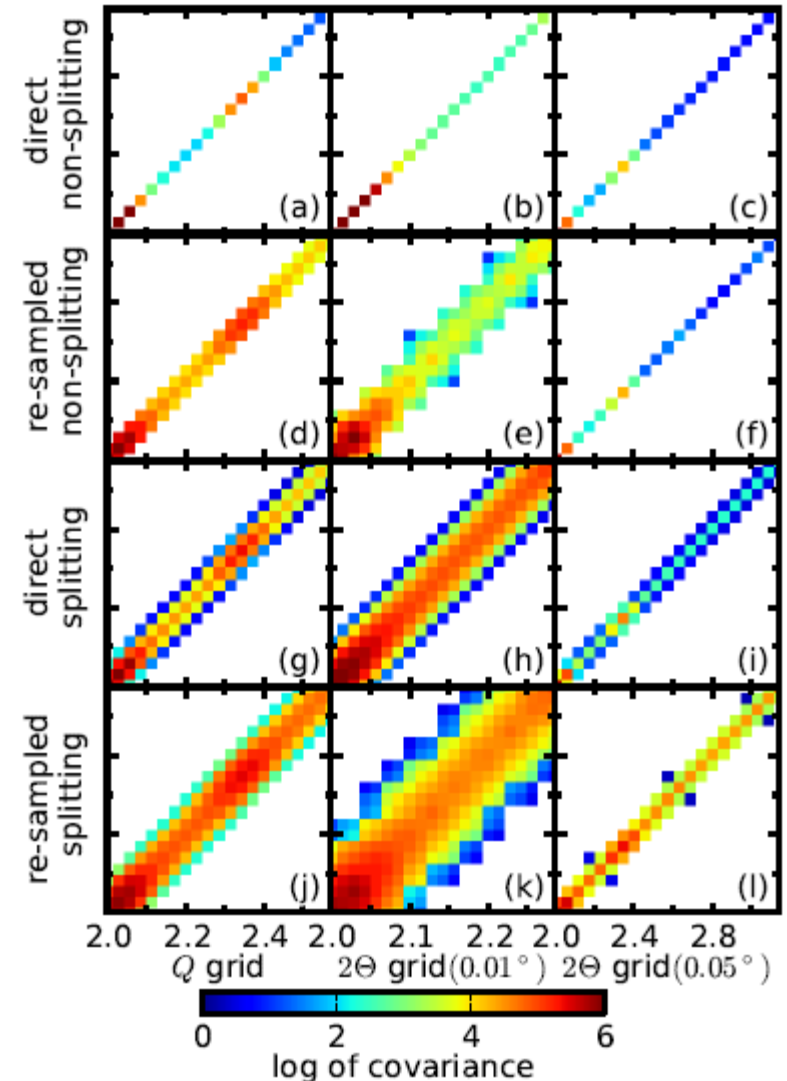


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- PDFgetX2, GudrunX

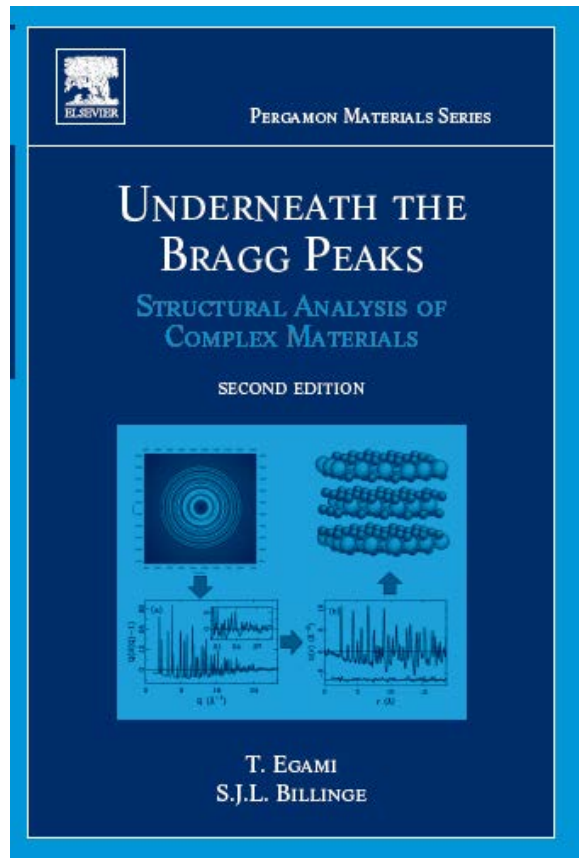
## An aside: estimating uncertainties from 2D detectors

- Not easy
- Lots of “black art” but not much rigor
- Current workflow:
  1. Use the default on Fit2D (pixel splitting)
  2. Hope for the best
  3. Publish some kind of error bars that you make up
- Advert for Xiaohao Yang’s work: we are considering esd estimation on the raw data and statistical correlations on data
- Variance-Covariance matrices for different common integration and interpolation schemes



# Data reduction to get the PDF

- Traditional Approach, apply all the physical corrections:



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- PDFgetX2, GudrunX

## Data Corrections

$$\left(\frac{d\sigma^s}{d\Omega}\right) = \int \left(\frac{d^2\sigma^s}{d\Omega dE_s}\right) W(E_s) dE_s$$
$$= \left[ \left(\frac{N}{M}\right)^{sc} - \left(\frac{V'_{c;sca}}{V'_{c;ca}}\right) \left(\frac{N}{M}\right)^c \right] \left( \frac{1}{\rho^s V'_{s;sca} D d\Omega K \epsilon_d} \right) - m'$$

- Underneath the Bragg Peaks, Chapter 5
- PDFgetX2, GudrunX.....
- GSASII

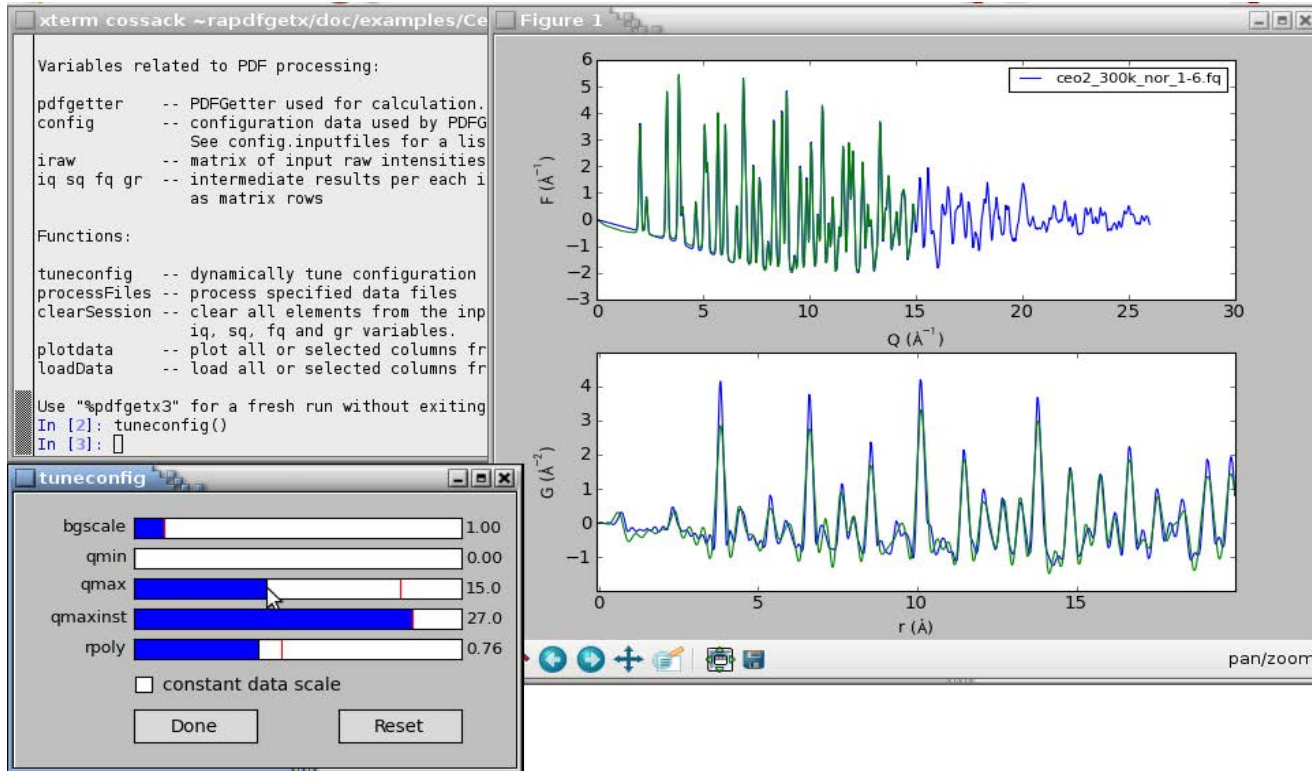
## Or treat the data reduction as an inverse problem

$F(Q)$  can be expressed in a general form as a function of the measured powder diffraction intensity:

$$F(Q) = \alpha(Q)I_m(Q) + \beta(Q)$$

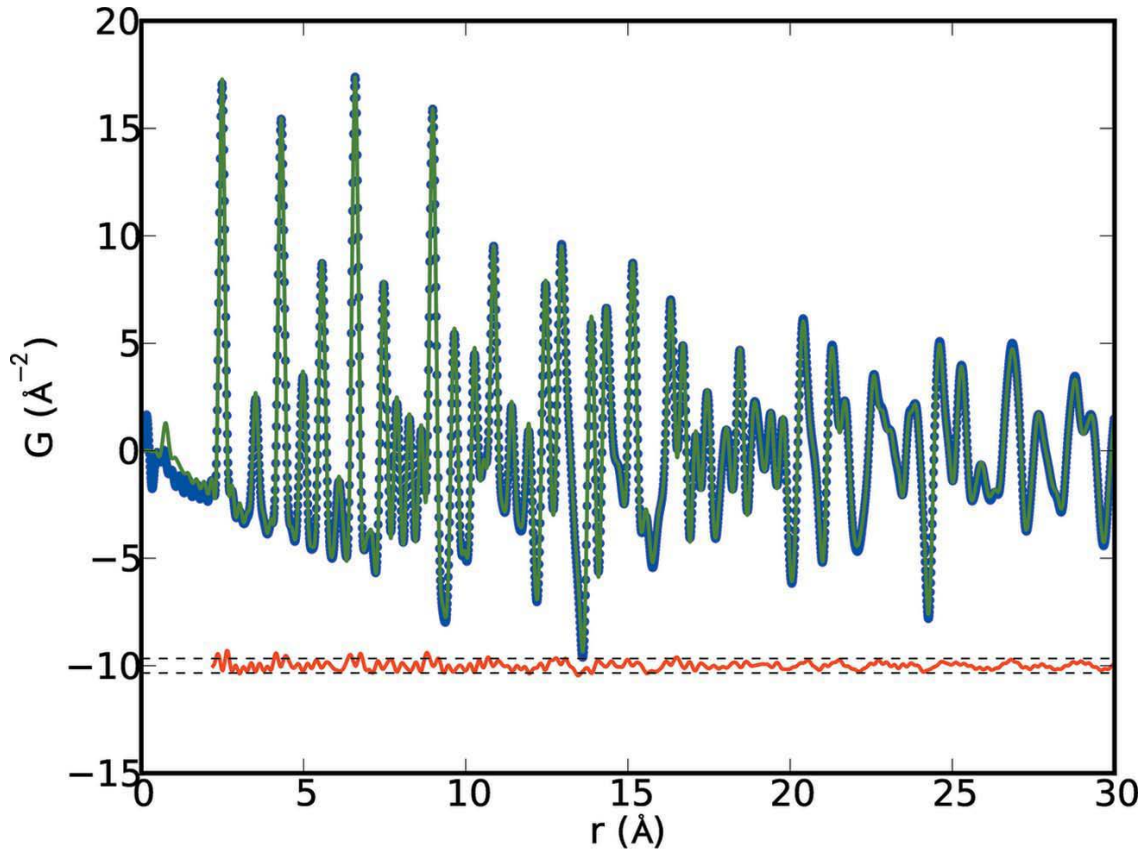
- Do we know enough about the form of alpha and beta and the asymptotic behavior of  $F(Q)$  to solve this in an ad hoc way?
- Answer is yes:
  - Billinge and Farrow, *J. Phys. Condensed Matter* (in press)
  - Juhas P., Davis T., Farrow C.L. and Billinge S.J.L., **PDFgetX3: A rapid and highly automatable program for processing powder diffraction data into total scattering pair distribution functions**, *J. Appl. Crystallogr.* **46**, 560-566 (2013).

# PDFgetX3 – conversion of powder data to PDF



- command-line application for extracting PDFs from X-ray powder data
- improved data-correction procedure → few process parameters, simple, easy to use
- automatable and fast – hundreds of PDFs processed within few seconds
- interactive parameters tuning with real-time plot updates
- scriptable from system shell or via Python interface included with the program

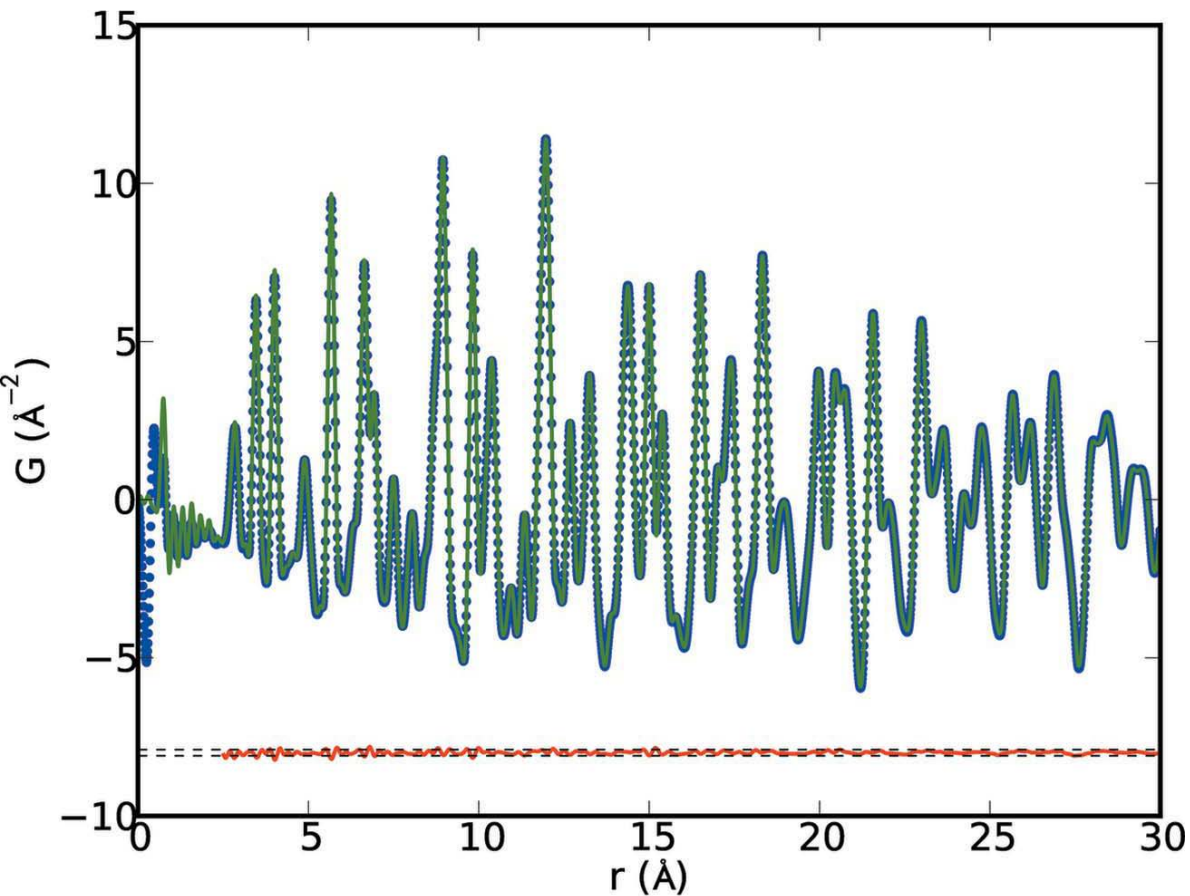
# PDFgetX3 comparison with PDFgetX2



- Green getX3
- Blue getX2
- Red difference
- Nickel

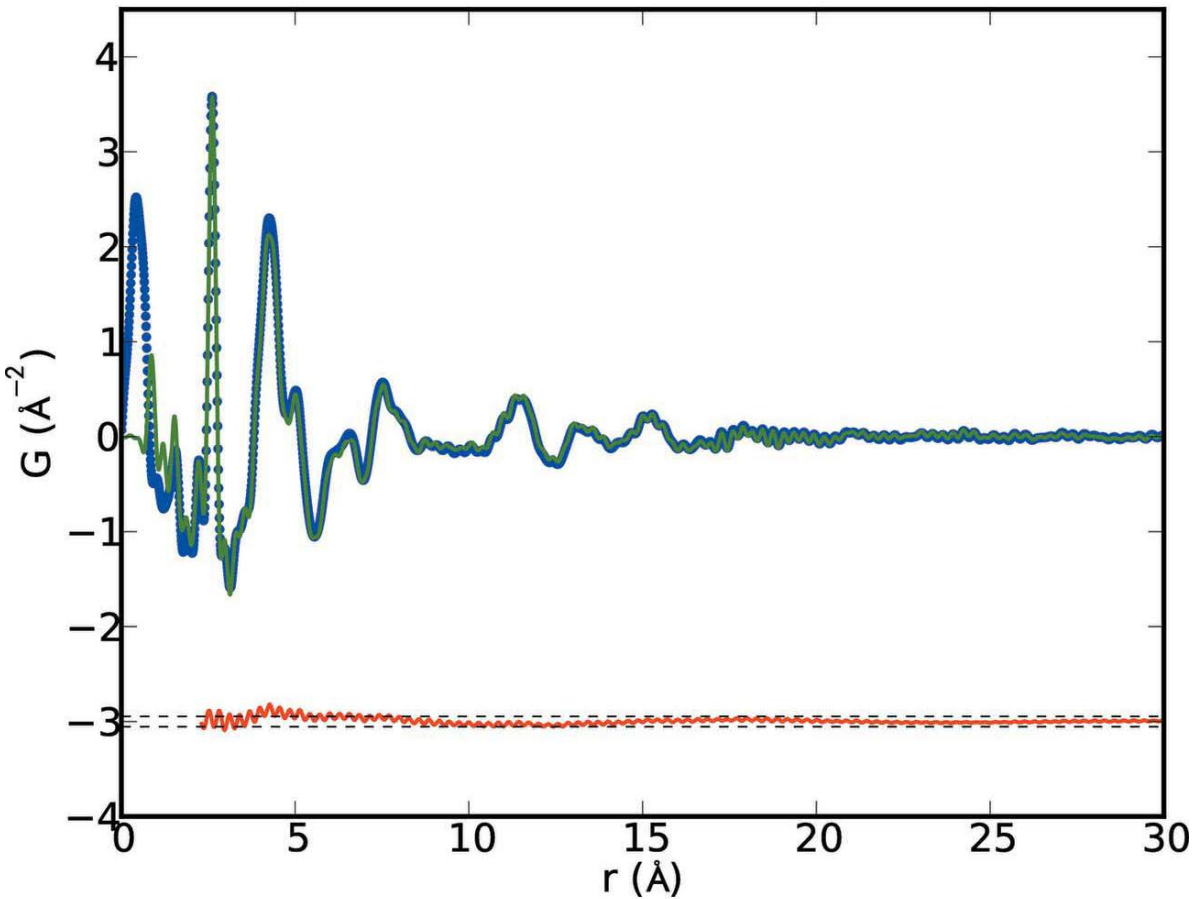


# PDFgetX3 comparison with PDFgetX2



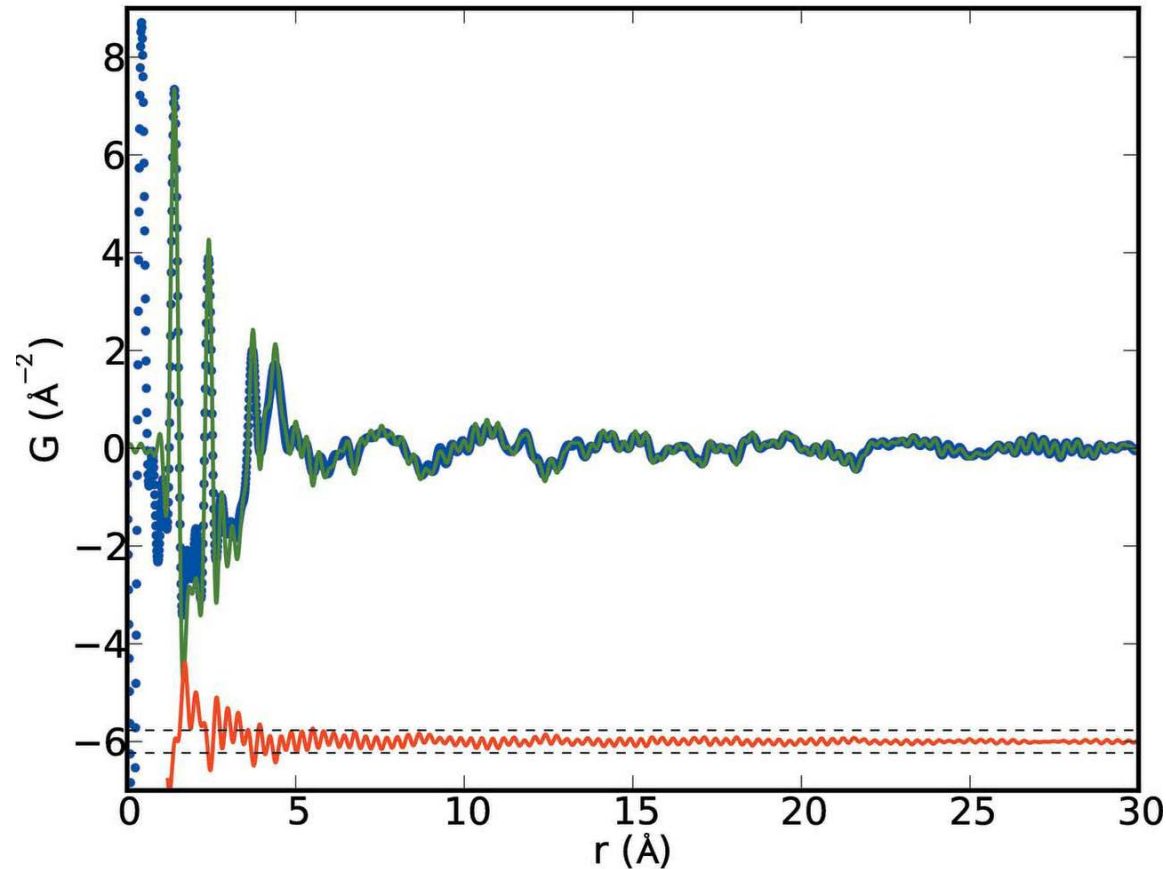
- Green getX3
- Blue getX2
- Red difference
- BaTiO<sub>3</sub>

# PDFgetX3 comparison with PDFgetX2



- Green getX3
- Blue getX2
- Red difference
- Ultra-small CdSe nanoparticles

# PDFgetX3 comparison with PDFgetX2



- Green getX3
- Blue getX2
- Red difference
- Nanostructured carbamazepine (pharmaceutical)

## Summary and outlook

- We now have amazing tools for collecting and analyzing data
- However...
- In complex materials modeling in general: we need more rigor
- Especially in Nanostructure modeling: we need more rigor
- Complex modeling is a first step
  - SrFit is our python-based complex modeling framework

In some sense, accuracy is the least of our problems:

actualcy is more the issue