FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
FACULTY OF SCIENCES

DISCUS

Simulation and refinement of disorderd crystal structures

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ADD 2026
January 13th, 2026

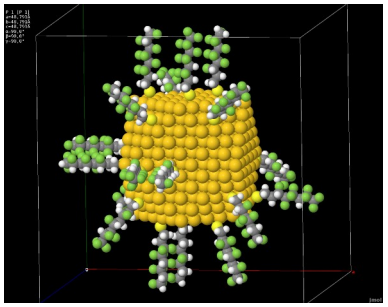
Small Box Modelling

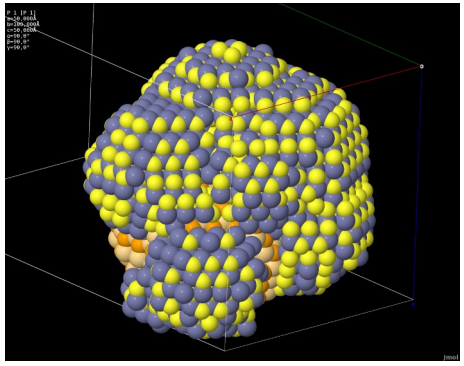
PDFgui

DISCUS
DiffPy

Large Box Modelling

Reverse Monte Carlo
RMCprofile
RMC_POT++
DISCUS



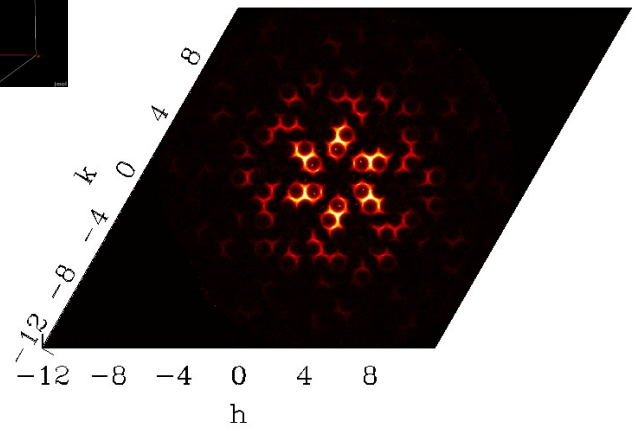


Multi level /
Complex Modelling

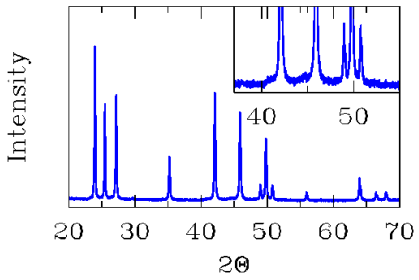
DISCUS
DiffPy

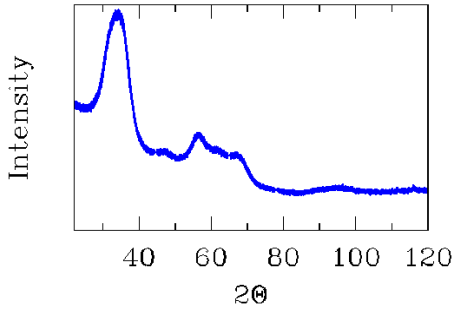
Single Crystal

DISCUS

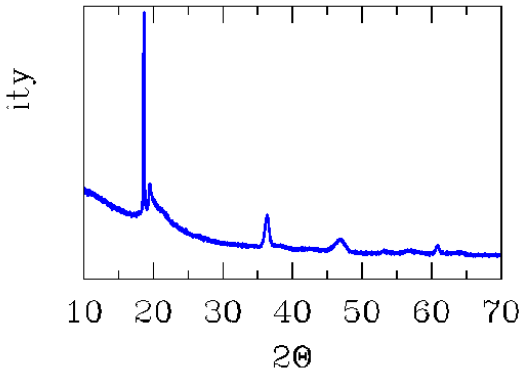


CdSe crystalline material



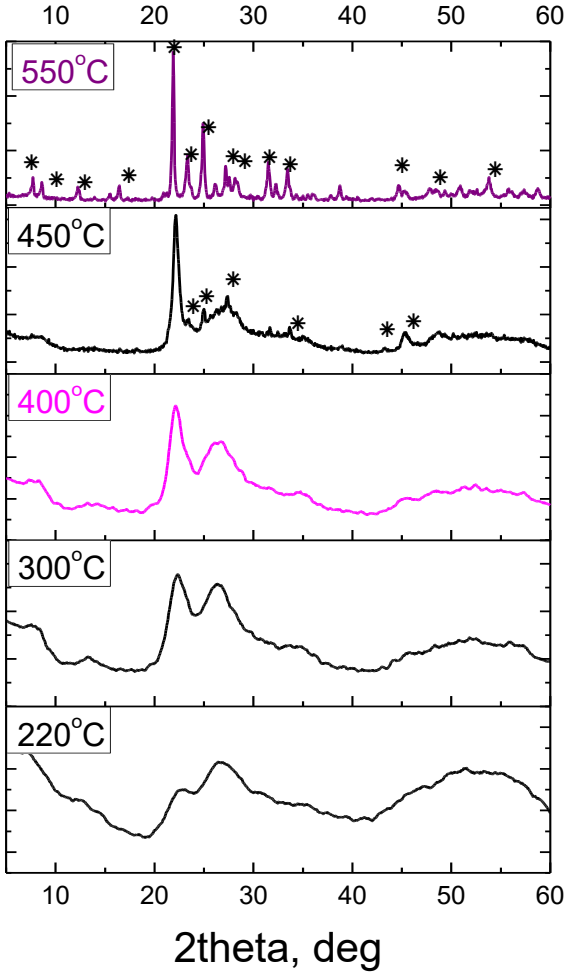


Nano crystalline ZnO



Massive stacking faults

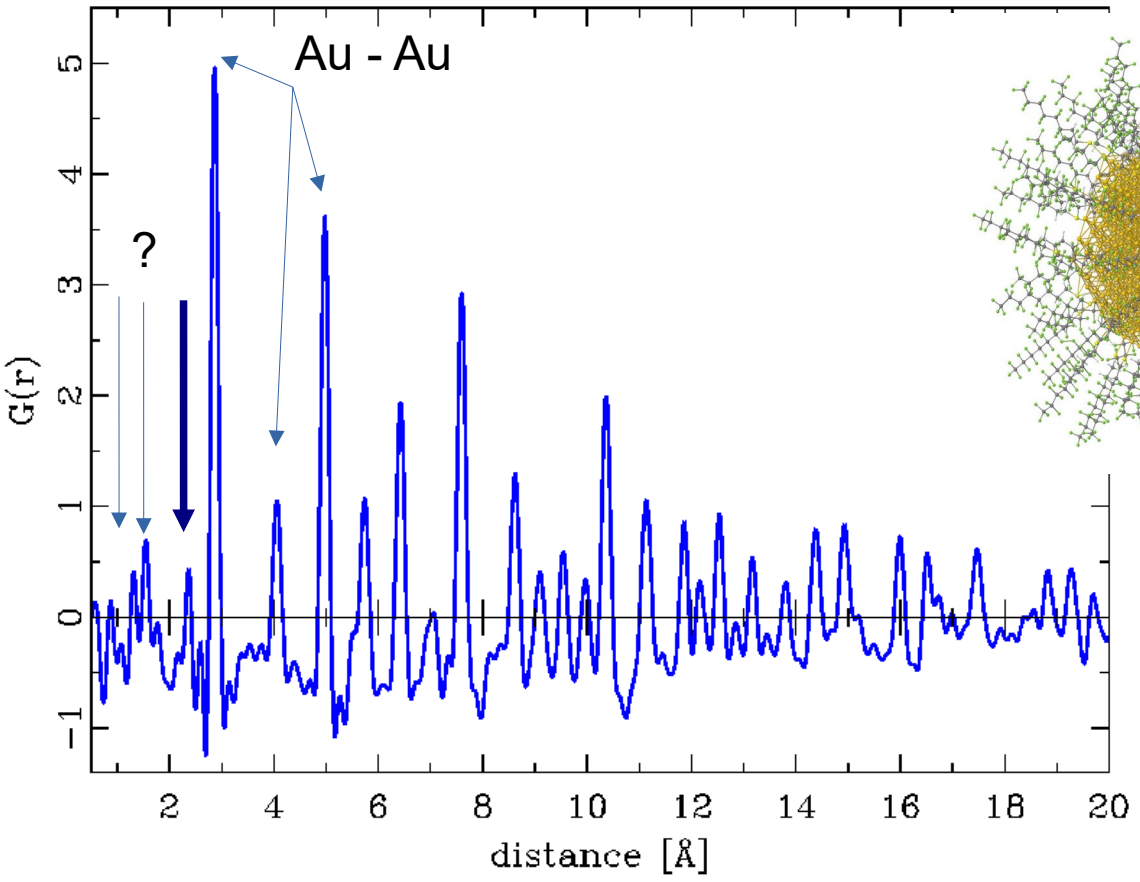
H_2TiO_3

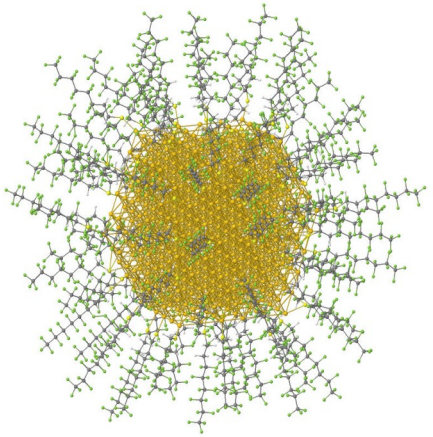


Mo-V-Nb oxides

Gold nanoparticles capped with fluorinated thio octane

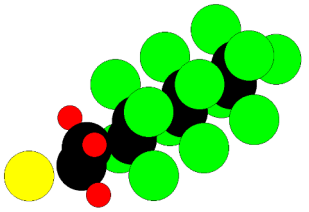
Gold -Ligand
Au – S 2.42 Å





Ligand -
Ligand
C-C 1.5Å
C-F 1.3Å

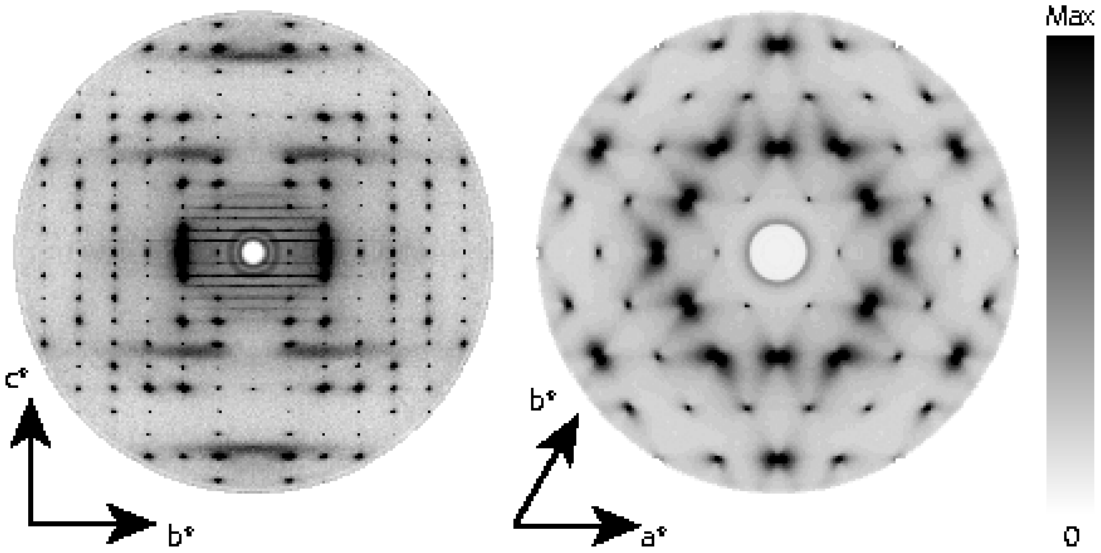
Number ?
Placement ?
Composition ?

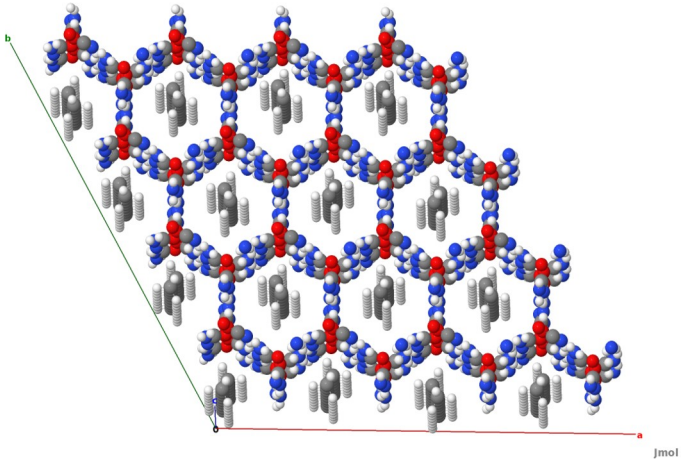


15 K
NPDF, Los Alamos
K. Page, Th. Proffen

K. Page et al. J.Appl. Cryst. (2011)

Th Weber PhD München 1994





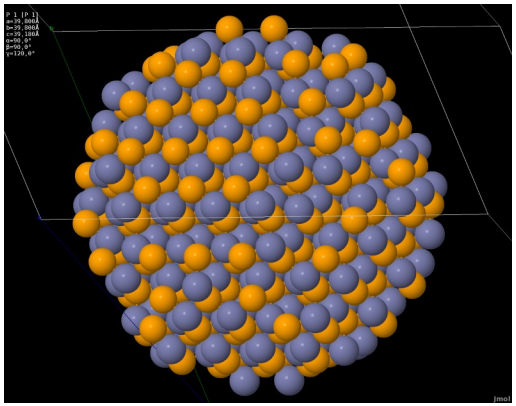
Alkane chains in Urea

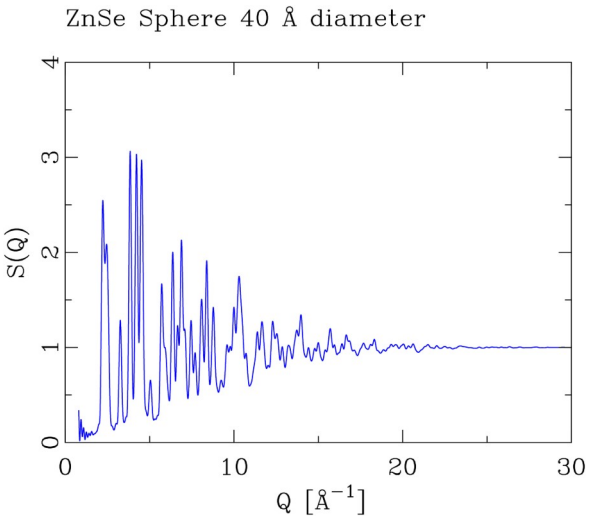
Diffuse scattering by 0.05 μm^3 single crystal
Neder et al Clays & Clay Minerals 1999

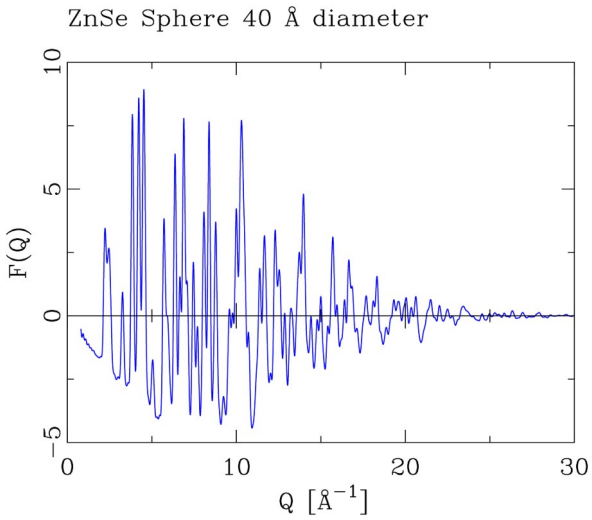
Welberry & Mayo J. Appl. Cryst 29, 1996

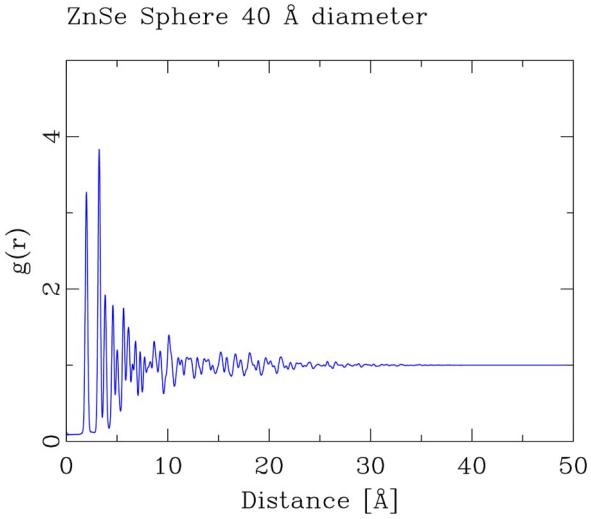
Simulate all sorts of nanoparticles

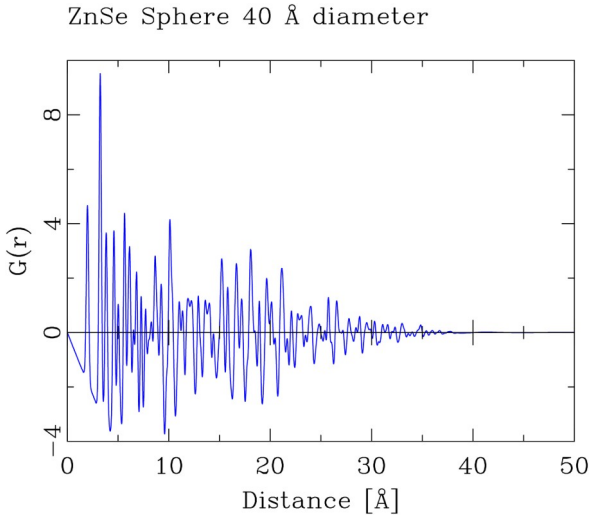
simple





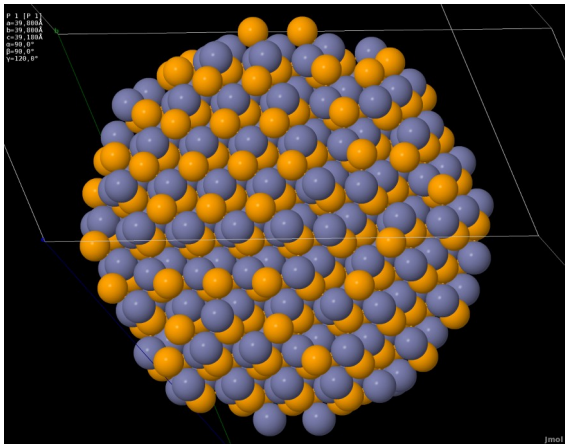




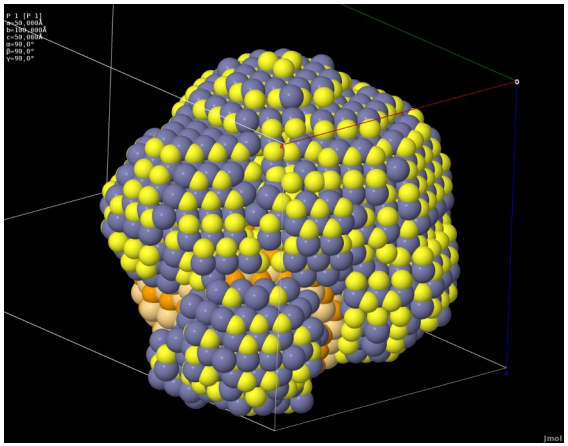


Simulate all sorts of nanoparticles

simple



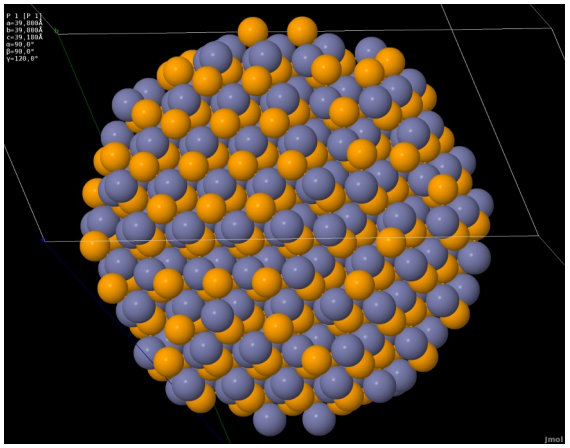
and complex



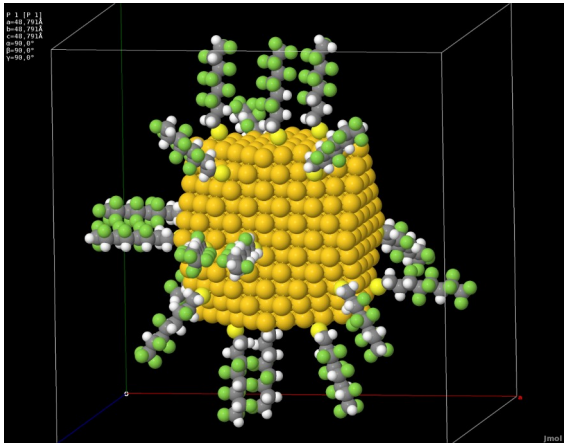
Build /shape
individual objects
Assemble into larger

Simulate all sorts of nanoparticles

simple

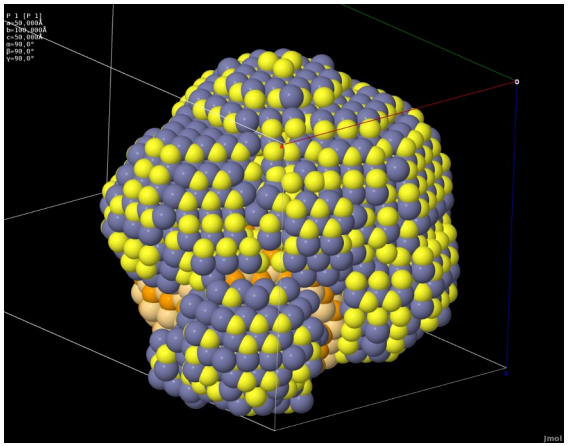


or decorated



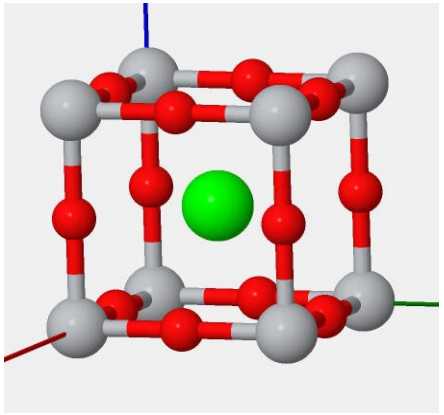
Shape core
Decorate

and complex

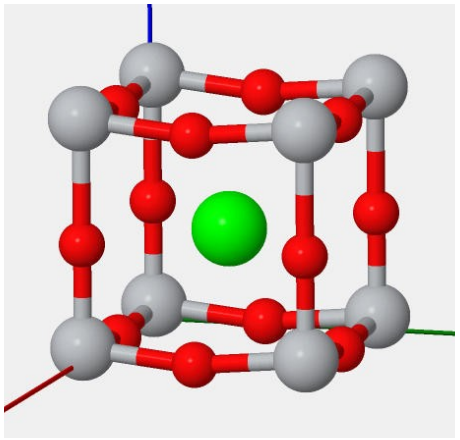


Build /shape
individual objects
Assemble into larger

Ideal Perovskite

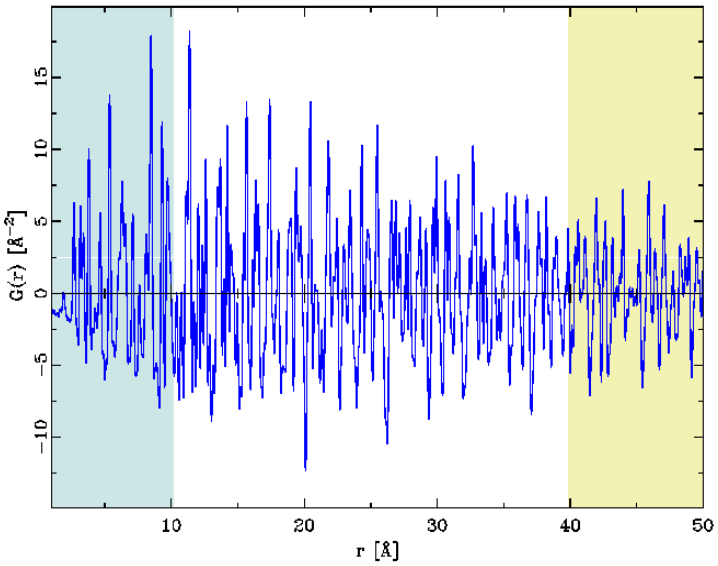


Shift Ti along [00z]

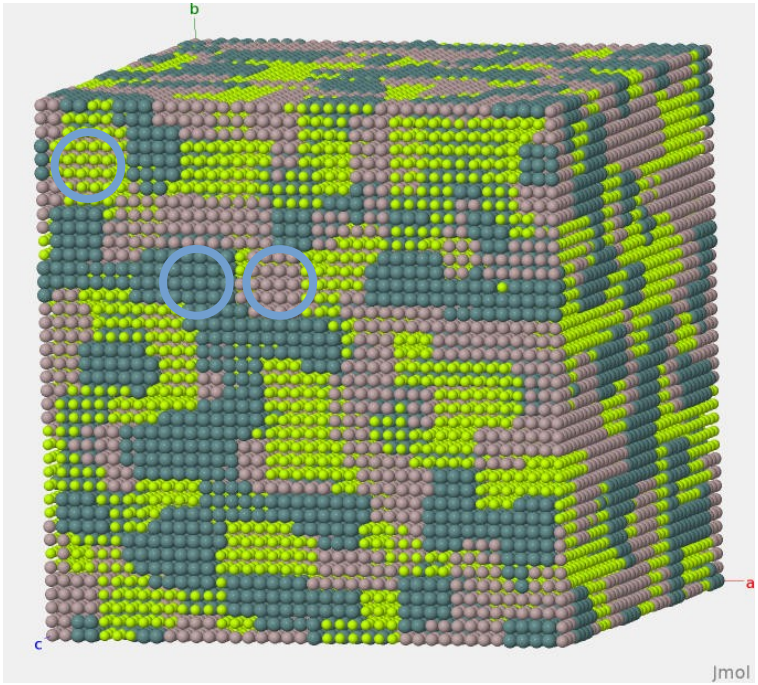


Three domains
[00z]
[0y0]
[x00]

***Experimental* G(r)**



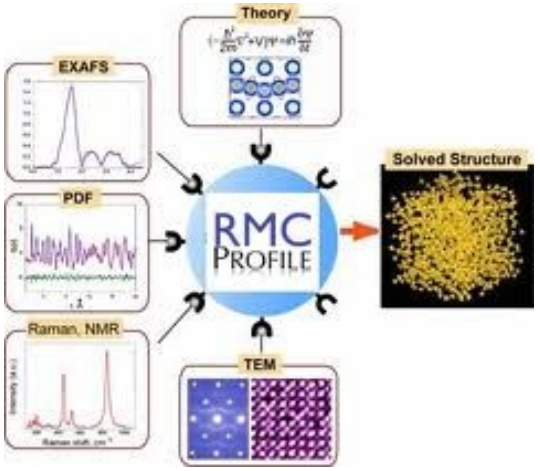
Focus on short distances



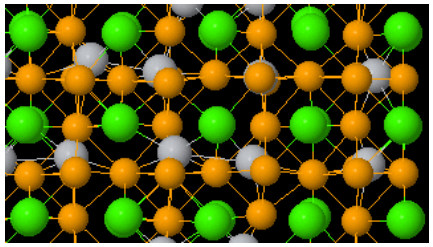
Small versus large box modeling

Large Box Modeling

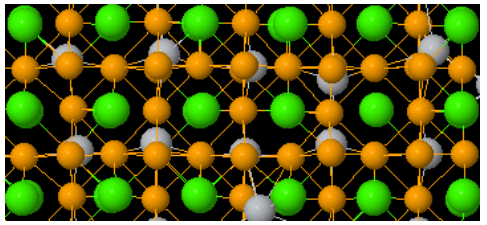
Reverse Monte Carlo
RMCprofile
RMC_POT++
DISCUS

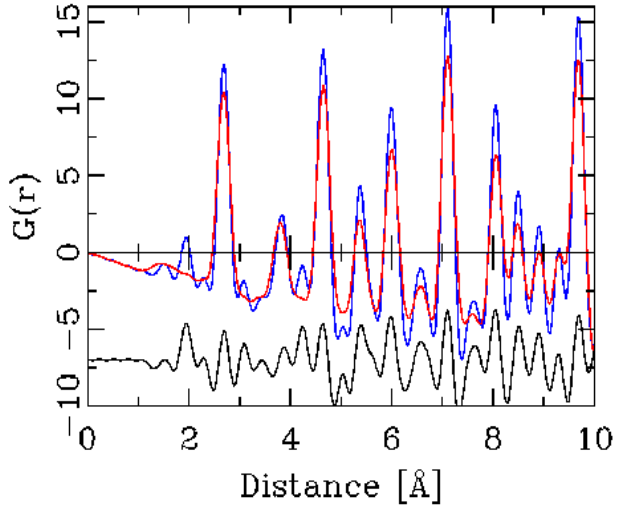


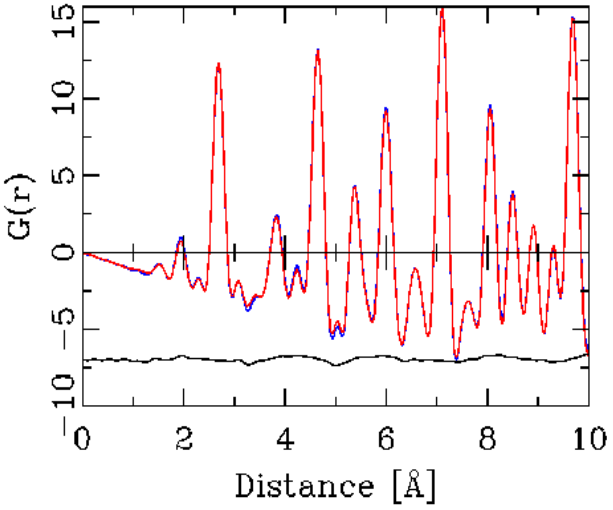
Model initial (random) **large** structure
Calculate PDF (+ powder + ...)



Modify structure (shift, exchange...)
while agreement improves
Usually requires constraints!



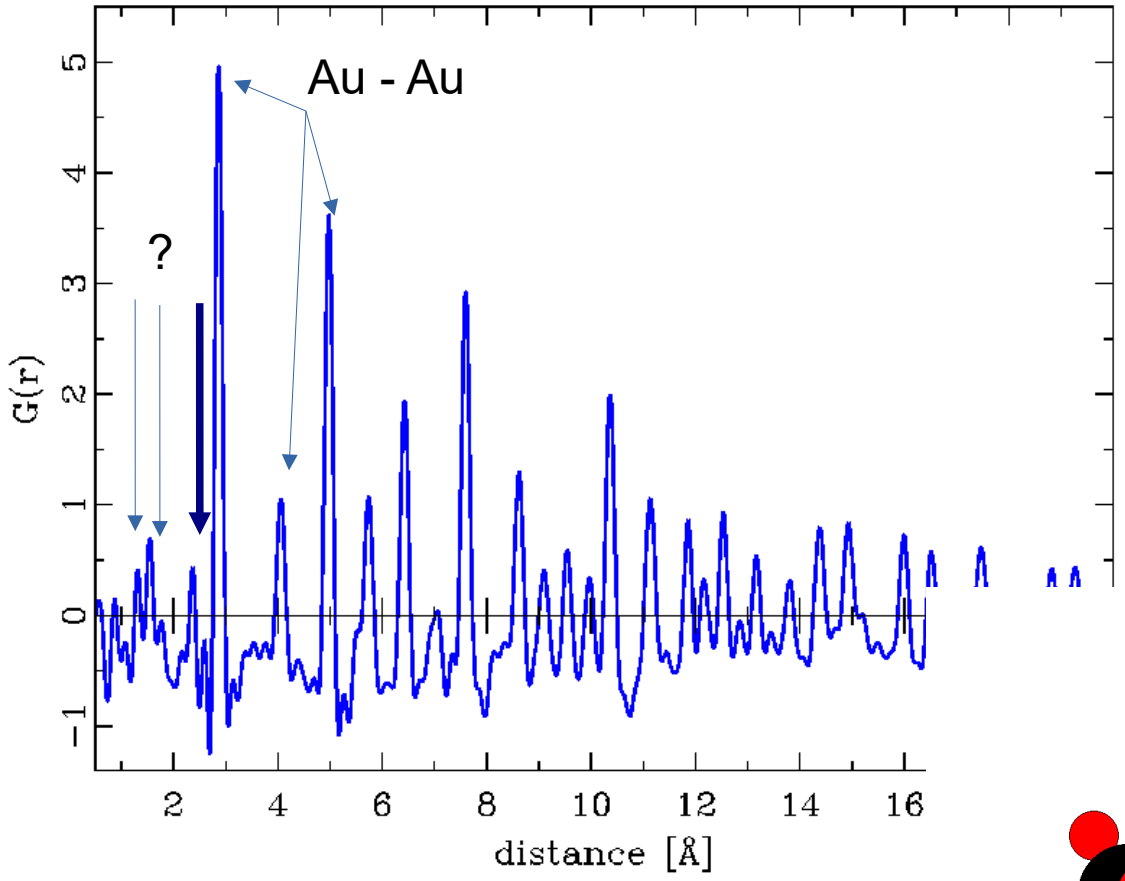




Nanoparticle + Ligand + Neutron Scattering

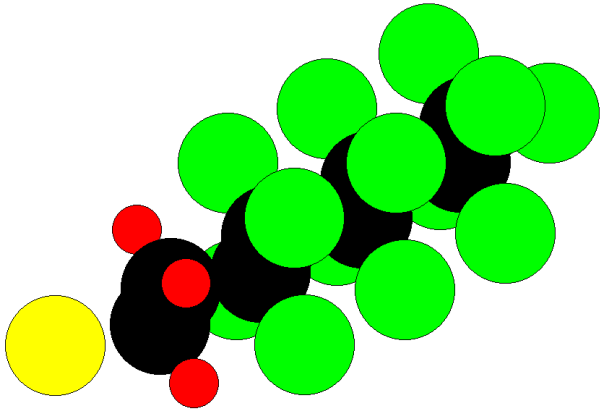
Gold -Ligand
Au – S 2.42Å

Ligand -
Ligand
C-C 1.5Å
C-F 1.3Å



Au
F m 3 m
a 4.064 Å
Au-Au 2.837Å

Number ?
Placement ?
Composition ?



15 K
NPDF, Los Alamos
K. Page, Th. Proffen, T. Cheetham

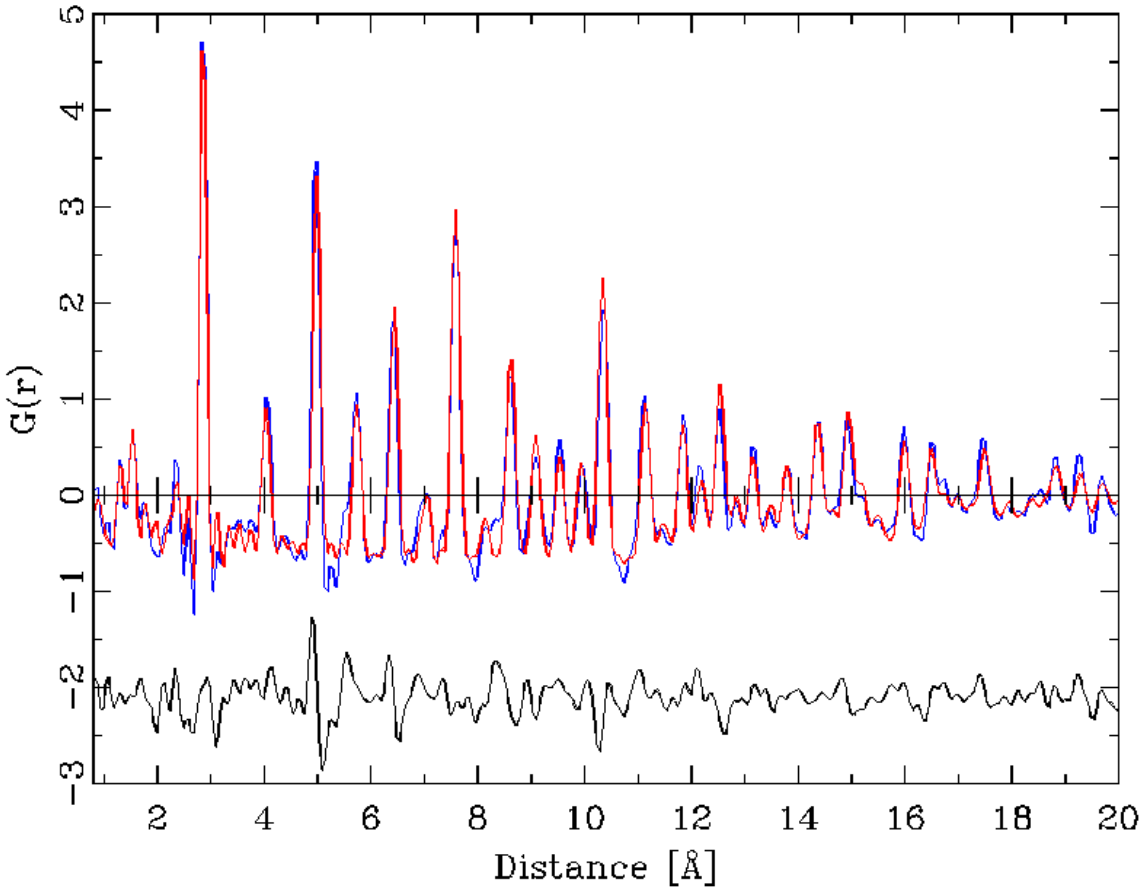
Au + S-CH2-CH2-(CF2)5-CF3

$S\ C_8\ H_4\ F_{13}$

Ligand internal distances
from DFT calculations

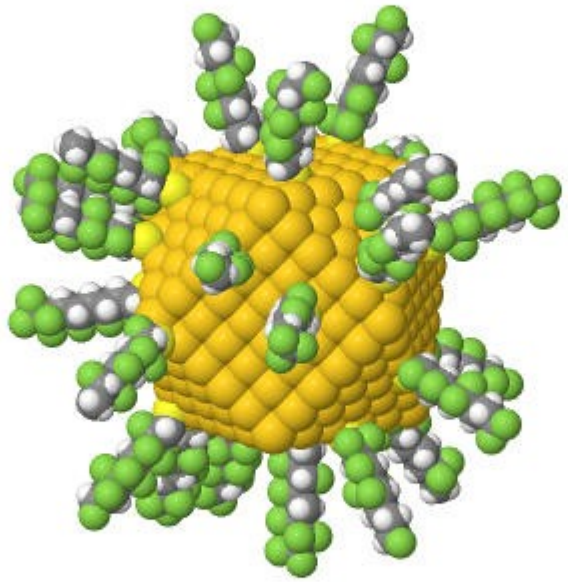
Page, *et al.*, *Chem. Phys. Lett.* **393** (2004) 385-388.

Nanoparticle + Ligand + Neutron Scattering



15 K
NPDF, Los Alamos

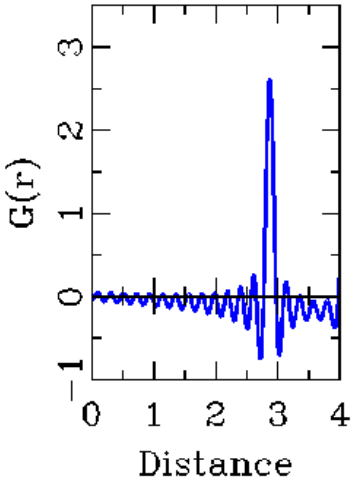
a(Au)	4.0658Å	(1)
Au – Au	2.8750Å	(1)
B(Au)	0.32Å^2	(4)
B(Ligand)	0.45Å^2	(10)
Diameter	20Å	(2)
N(ligand)	20	(6)
P(Fluorine)	0.65	(15)
Au – S	2.42 Å	fixed!



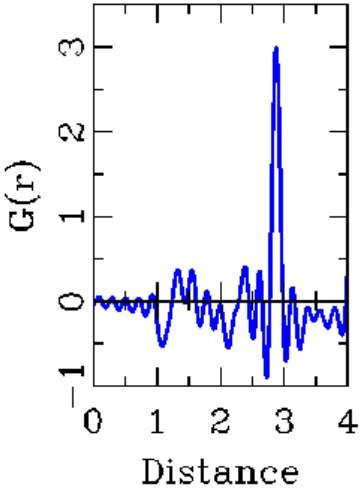
K. Page et al. J. Appl. Cryst. (2011)

Direct or not direct

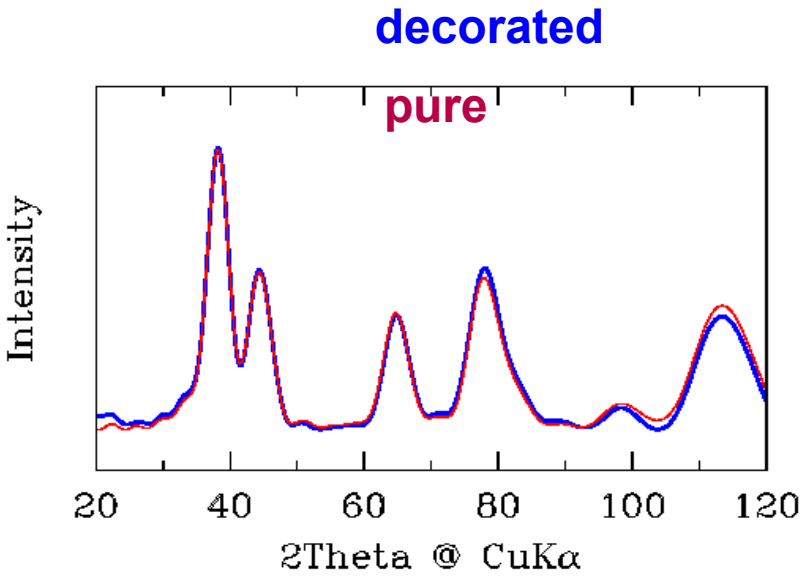
PDF

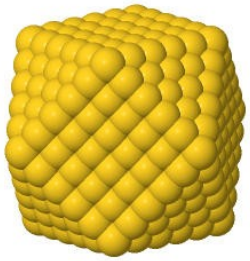


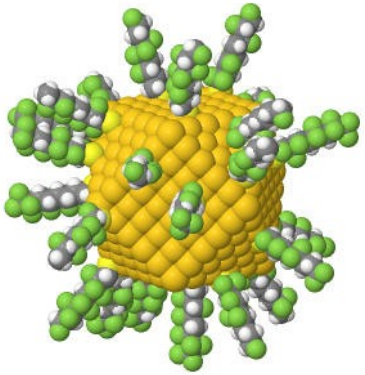
PDF



Calculated Debye-Scattering-Equation



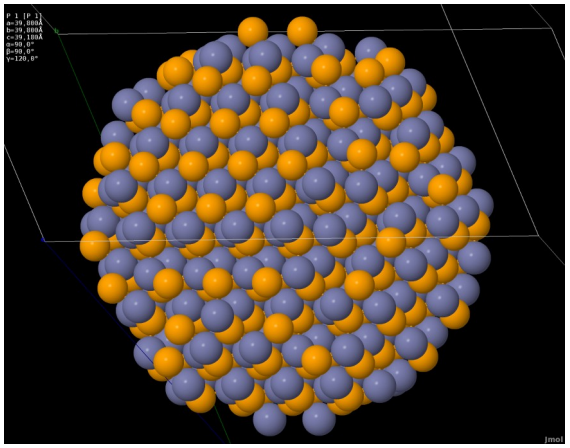




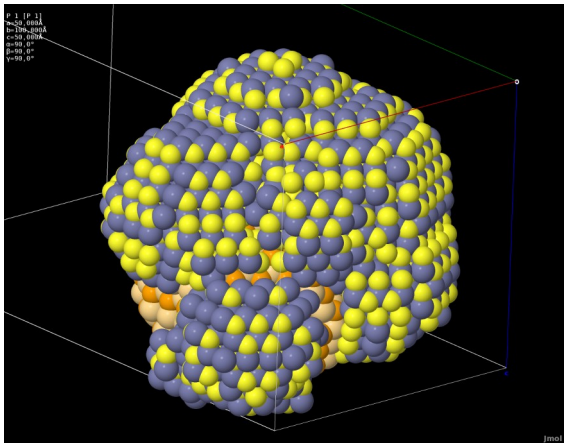
Essentially no *modulated* difference in NEUTRON powder diffraction pattern

Simulate all sorts of nanoparticles

simple

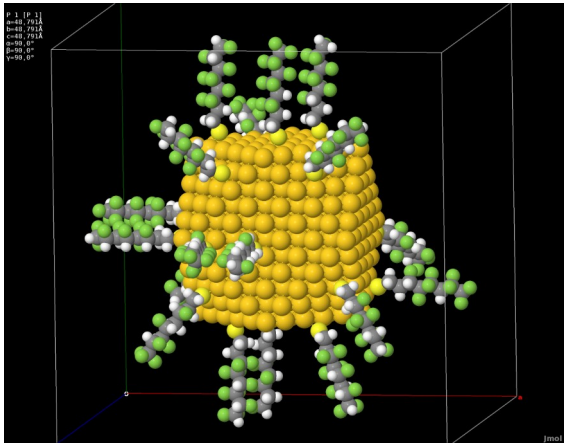


and complex



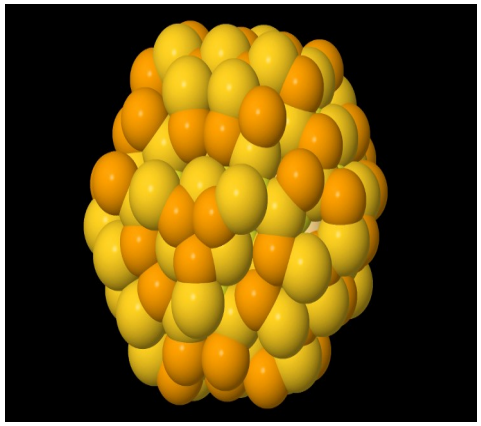
Build /shape
individual objects
Assemble into larger

or decorated



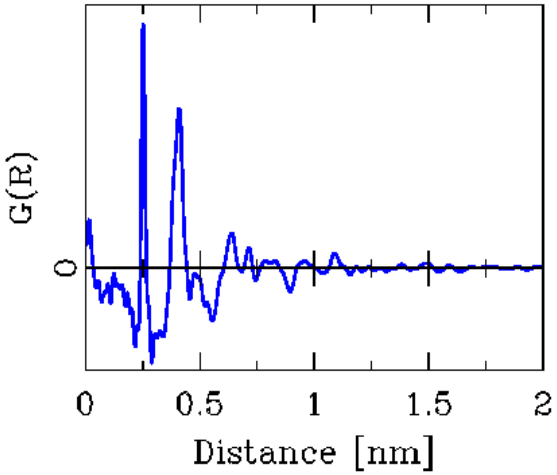
Shape core
Decorate

or distorted



Shape core
Distort
surface / core

CdS nanoparticles



CdS / Glutathione

Composition: $Cd_1\ S_{0.5}\ Glutathione_{0.5}$

Raman: No H-S vibration

All organic sulfur bound to CdS surface

Half surface S

Half core S

1.5 to 2 nm diameter

Korsounksi et al. J. Appl. Cryst. (2003), **36**, 1389

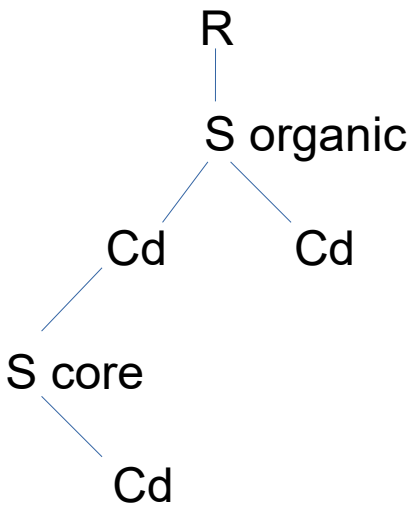
Strain determined by Ligand molecule

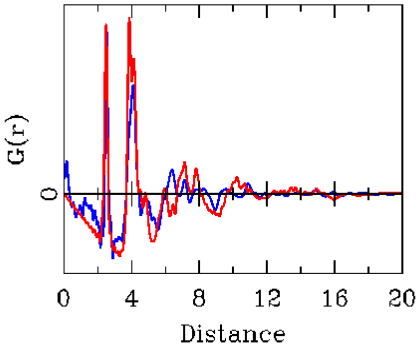
Different bond angles (distances) at surface / core

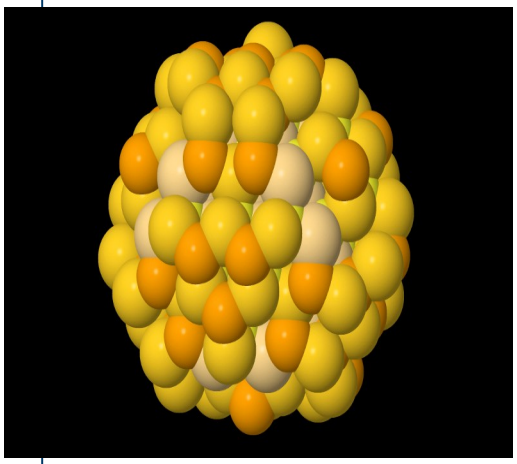
Inhomogeneous strain field across particle

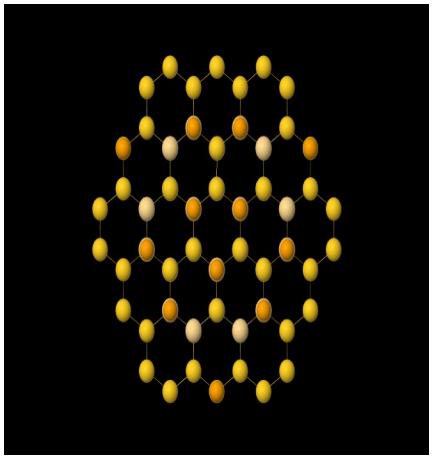
Relax particle to minimize energy

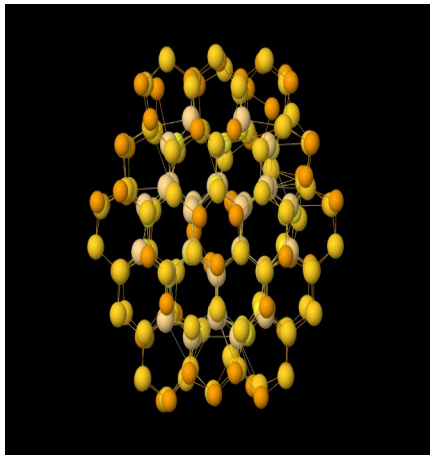
Potential: Cd – S (organic) – Cd angle
Cd – S (inorganic) – Cd angle
Cd – S first neighbor distance

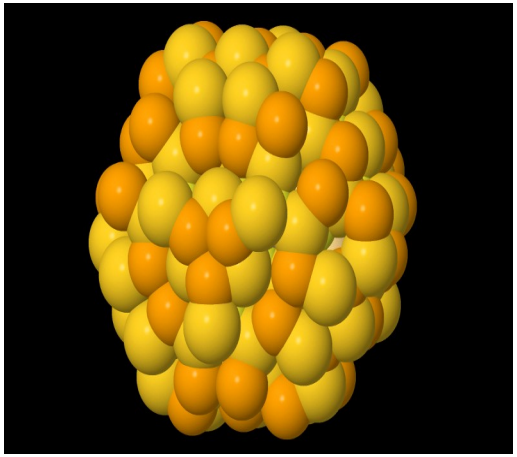








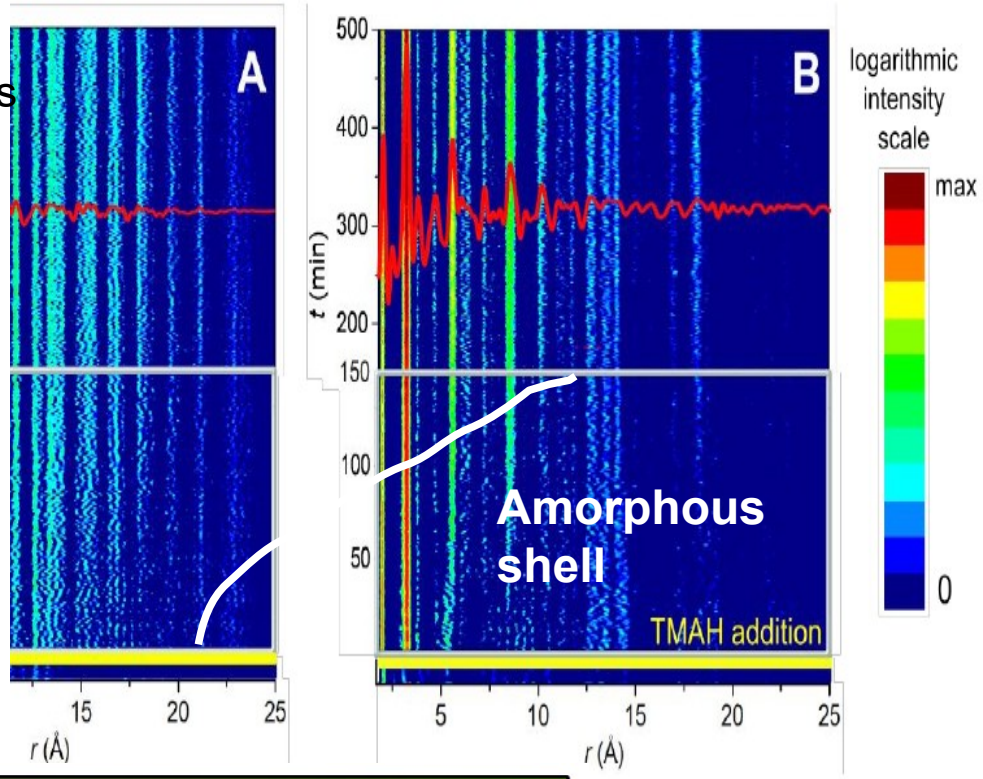


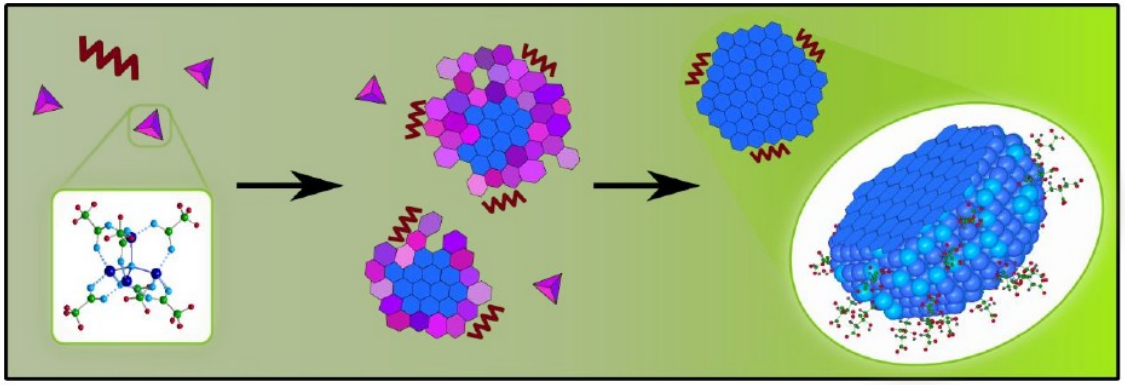


Not amorphous !

Nanoparticle interaction with Solvents

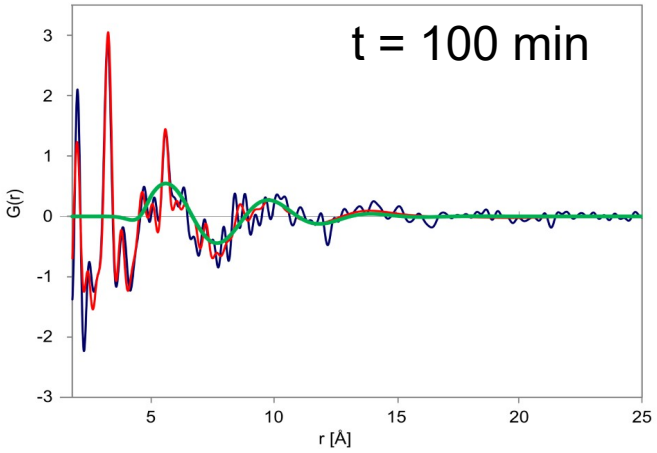
Initial formation of Zn-O precursor clusters
Rapid formation of disordered particles
Slow internal ordering of core structure

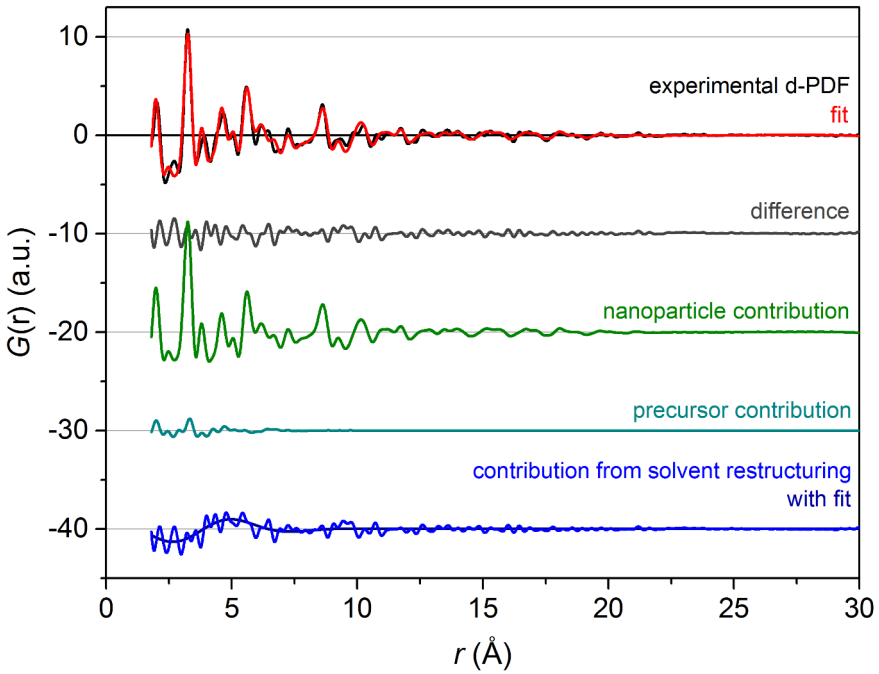




M. Zobel, A. Windmüller, …, R.B. Neder, (2016) Cryst.Eng.Comm, **18**, 2163

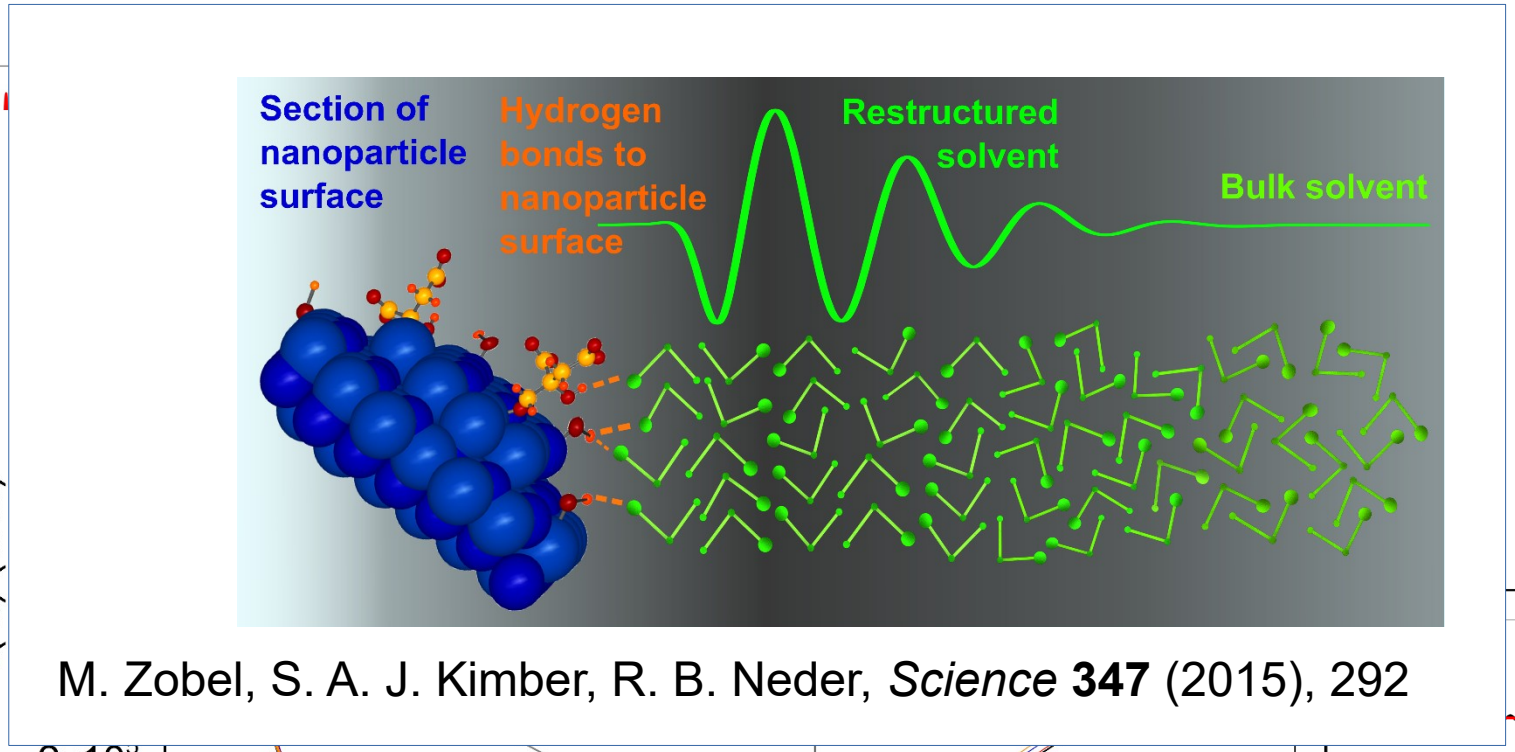
Nanoparticle interaction with Solvents





Additional dampened sinusoidal oscillation

Nanoparticle interaction with Solvents



M. Zobel, S. A. J. Kimber, R. B. Neder, *Science* **347** (2015), 292

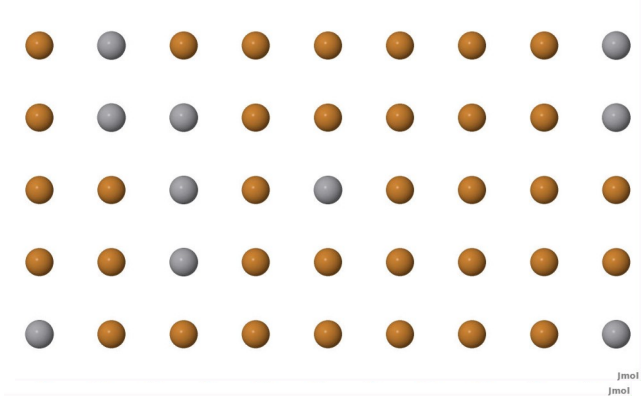
Read asymmetric unit

Expand to full unit cell
Expand to a block sized crystal

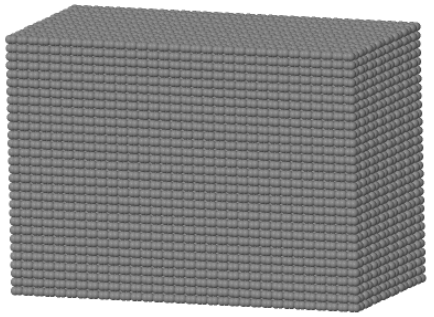
Modify crystal

Introduce defects

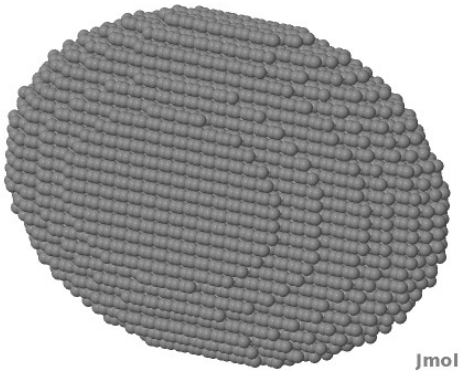
Extended tool box to introduce arbitrary defects



Modify crystal shape



Calculate: **single crystal diffraction pattern**
powder diffraction pattern
Debye-Scattering-Equation
Complete integration
powder PDF
3D Δ PDF

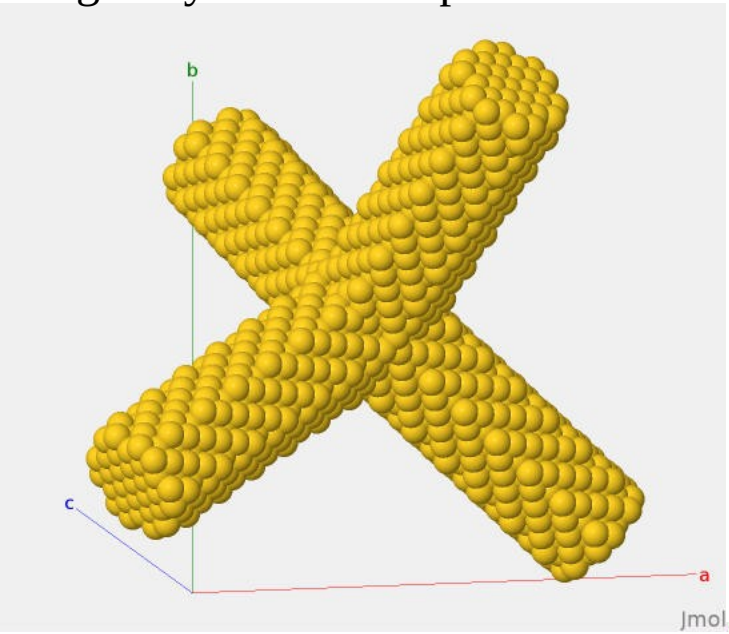


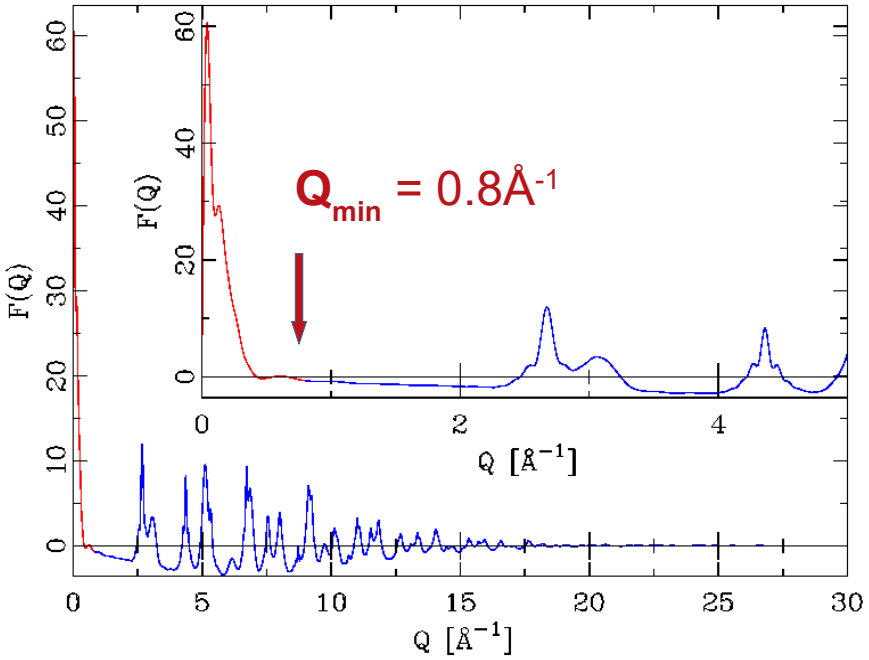
Xray, neutron, electron

Refine: structure and disorder
against experimental pattern

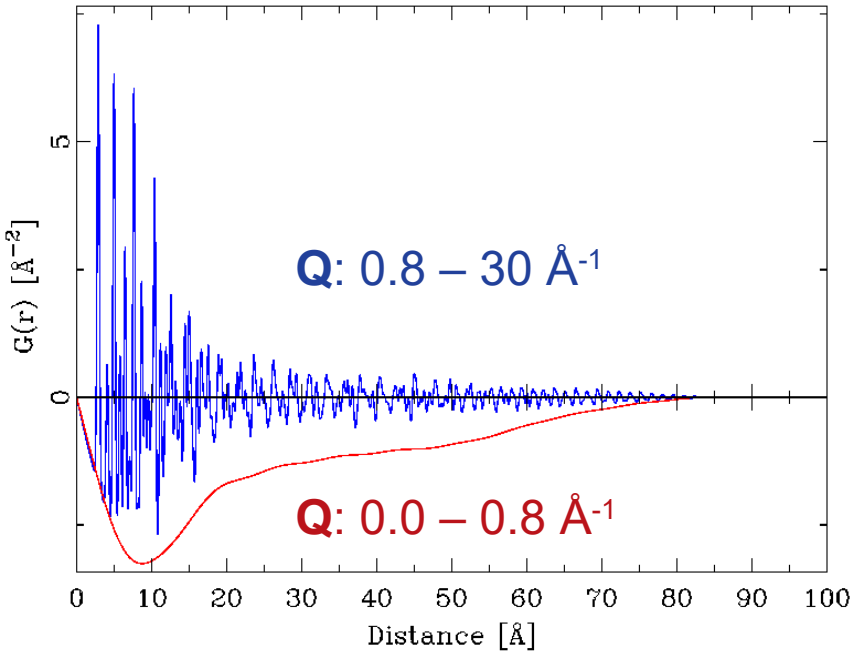
Complex Nanoparticle shape

Single crystal Au tetrapod





PDF as Fourier of diffraction pattern



Baseline as Fourier of
-1 * small angle scattering signal

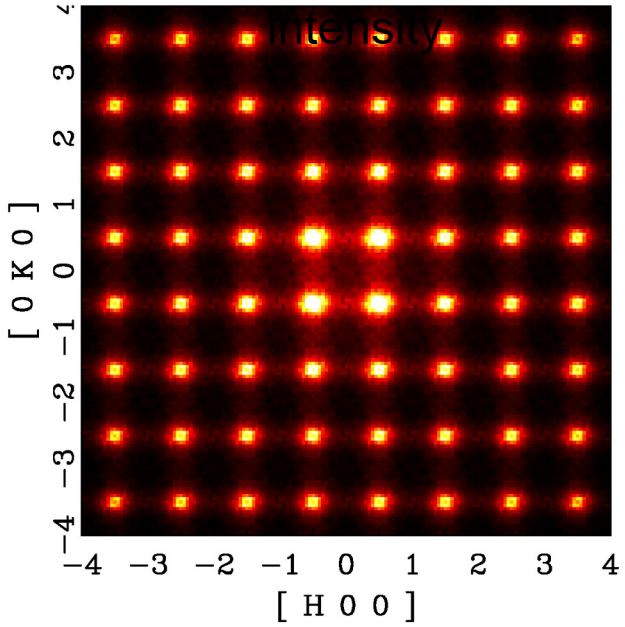
Neder & Proffen (2020) J.Appl. Cryst. **53**, 710

Calculation of 3D (Δ)-Pair Distribution Function PDF

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
FACULTY OF SCIENCES

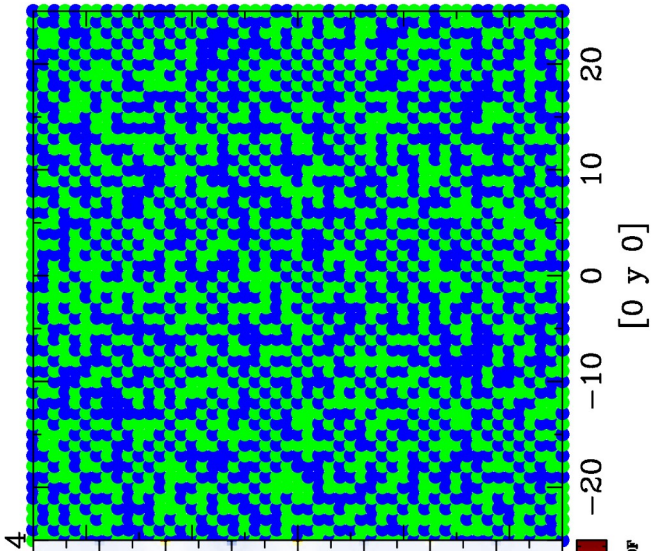
Calculation of 3D-PDF 3D-Delta-PDF from structural model

Diffuse intensity

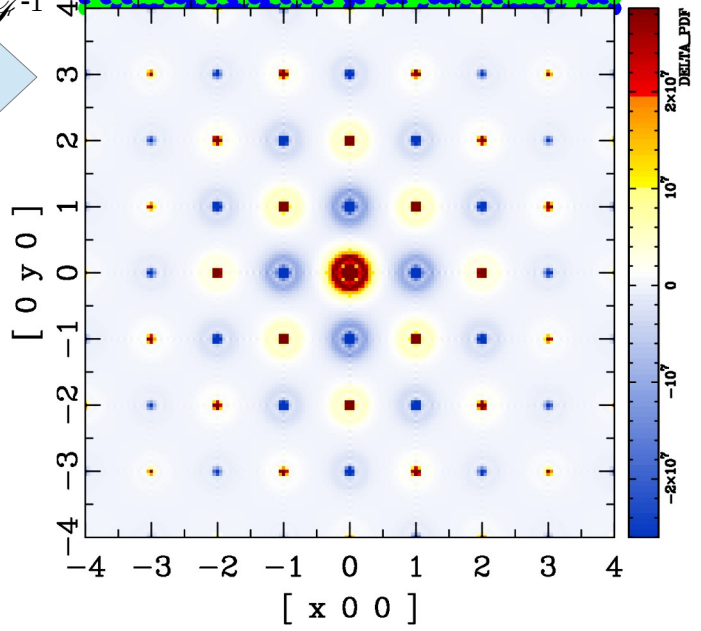


$\mathcal{F}$

Structure



$\mathcal{F}^{-1}$

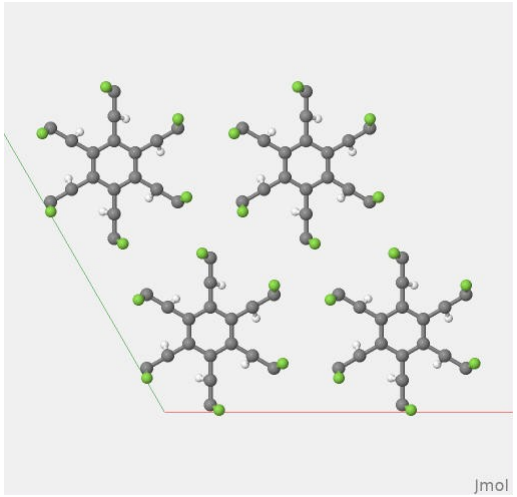


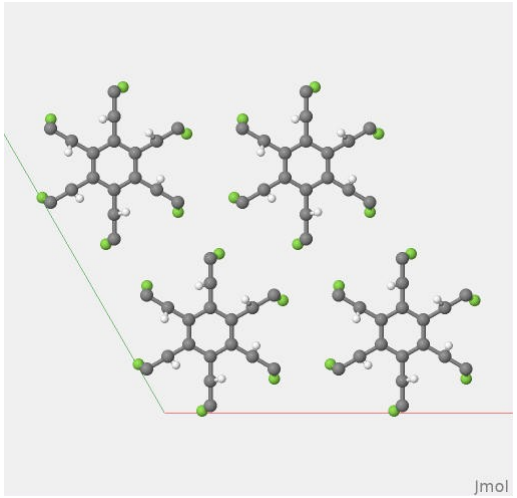
3D-ΔPDF

C100 target/achieved/−0.35 −0.33
C010 target/achieved/−0.35 −0.37
C110 target/achieved 0.20
CM10 target/achieved 0.21
temperature 1.5
Nickel : Palladium 0.50 : 0.50

Example

Columnar structure





Perfectly ordered **up**

Perfectly ordered **down**

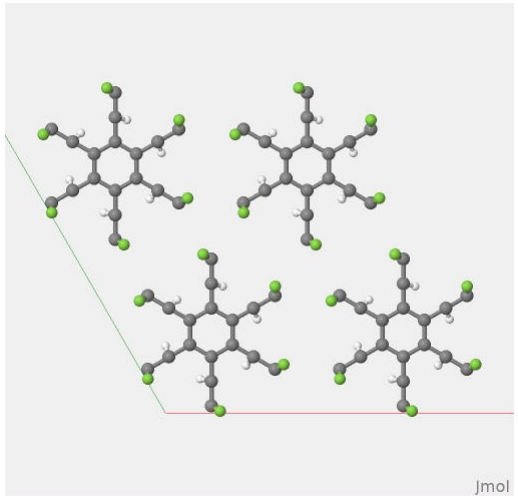
Target:

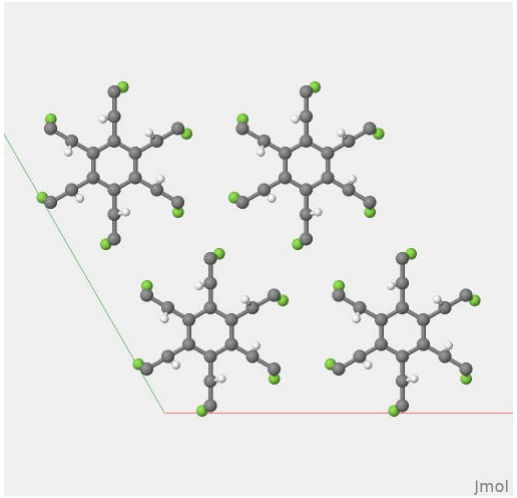
Perfect 6_3 order along c-axis

Negative correlation in a-b plane along
[1 0 0]; [0 1 1]; [1 1 0]

Example

Columnar structure



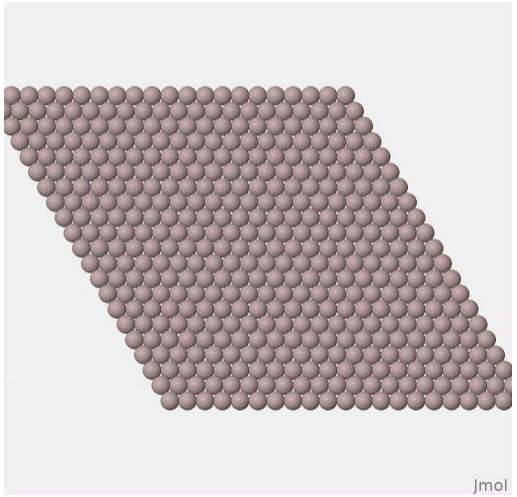


Perfectly ordered **up**

Perfectly ordered **down**

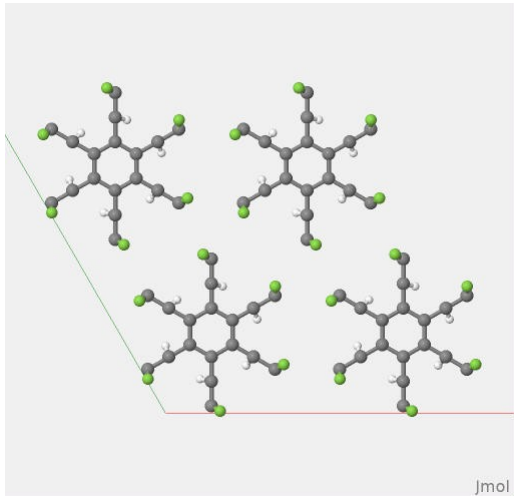
1st step

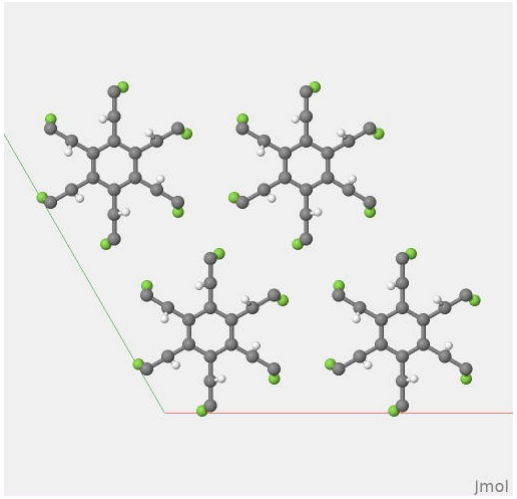
Create 2D crystal of dummy atoms “**A**“



Example

Columnar structure





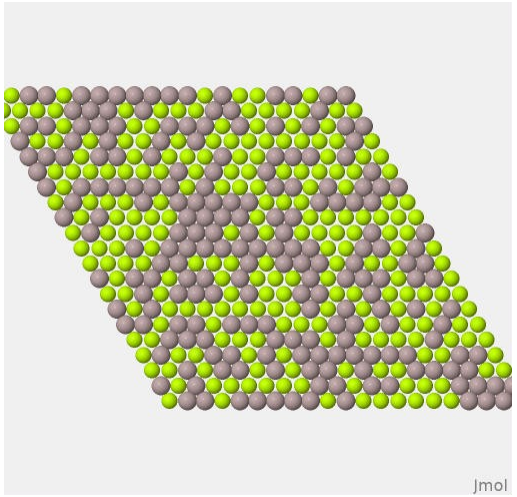
Perfectly ordered **up**

Perfectly ordered **down**

1st step

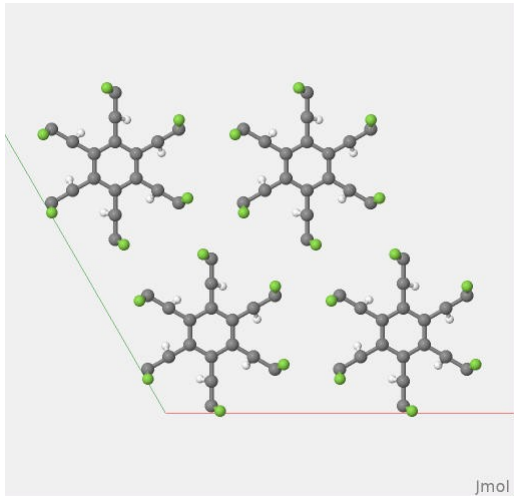
Create 2D crystal of dummy atoms “**A**“

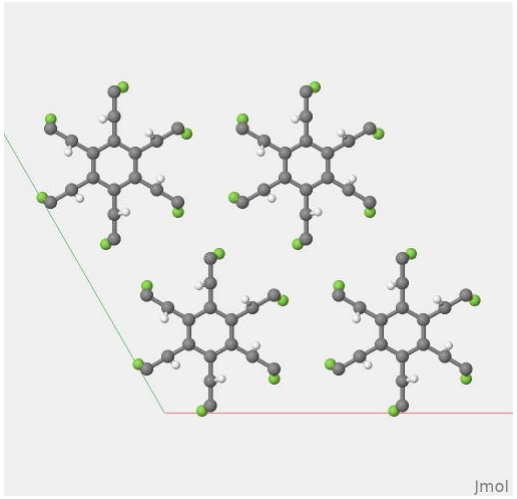
Replace 50% “**A**“ by “**B**”



Example

Columnar structure





Perfectly ordered **up**

Perfectly ordered **down**

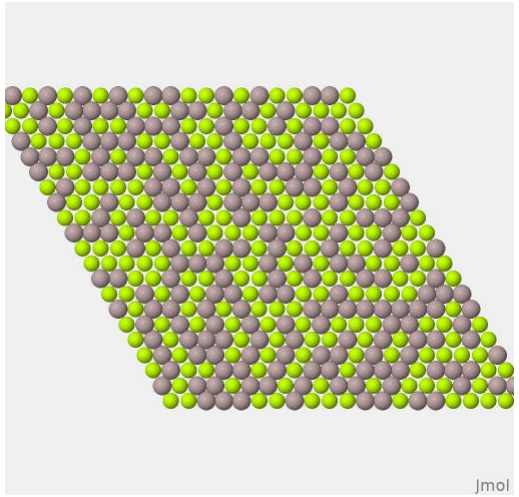
1st step

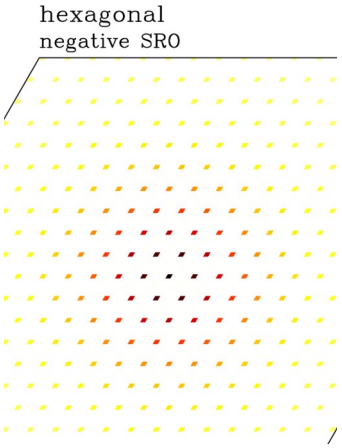
Create 2D crystal of dummy atoms “**A**“

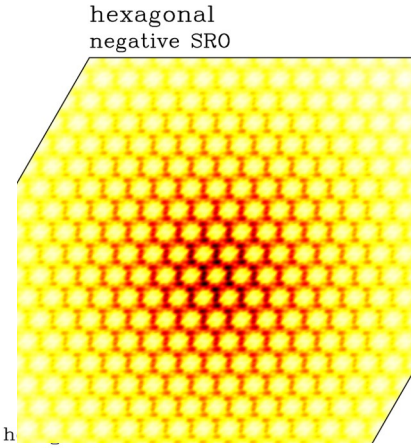
Replace 50% “**A**“ by “**B**”

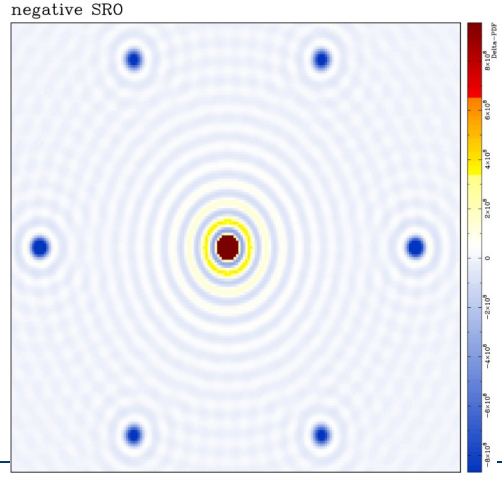
Sort “**A**“ and “**B**” with negative correlations

→ Hexagonal frustration!



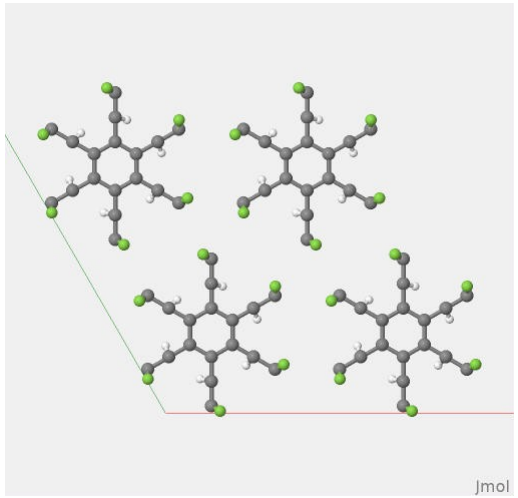


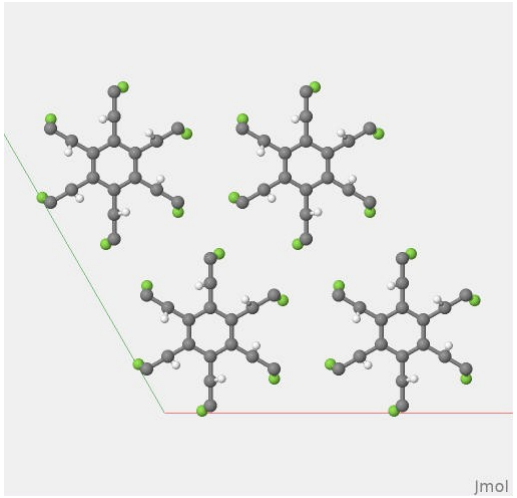




Example

Columnar structure





Perfectly ordered **up**

Perfectly ordered **down**

1st step

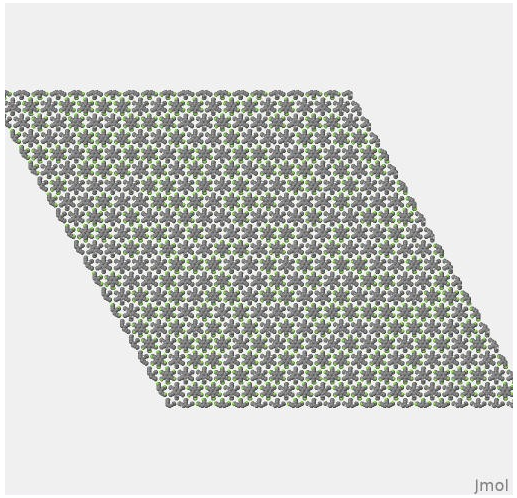
Create 2D crystal of dummy atoms "**A**"

Replace 50% "**A**" by "**B**"

Sort "**A**" and "**B**" with negative correlations

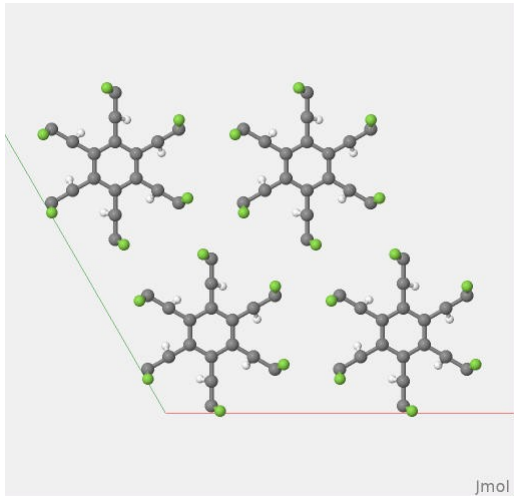
→ Hexagonal frustration!

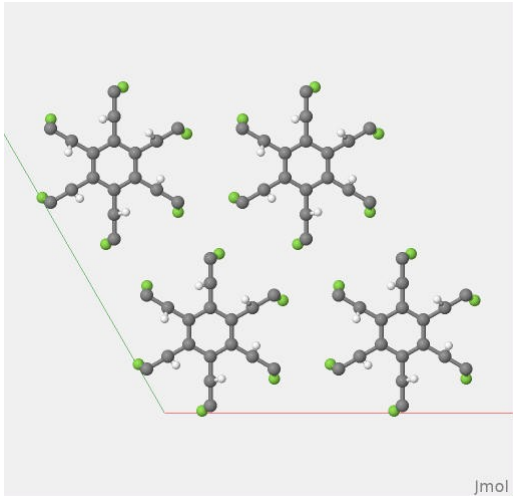
Replace "**A**" with **up** molecule and "**B**" with **down** molecule



Example

Columnar structure





Perfectly ordered **up**

Perfectly ordered **down**

1st step

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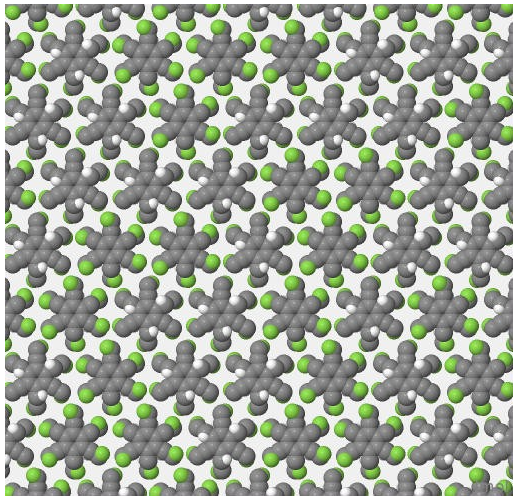
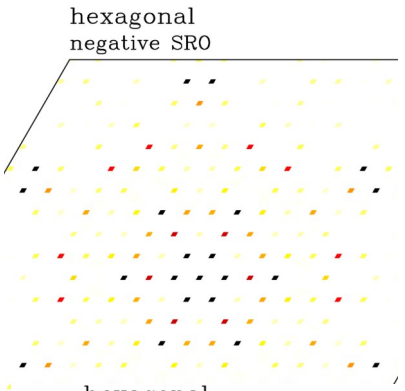
Replace 50% “**A**“ by “**B**”

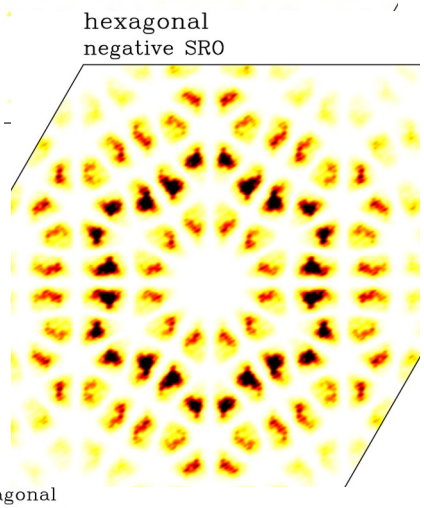
Sort “**A**“ and “**B**” with negative correlations

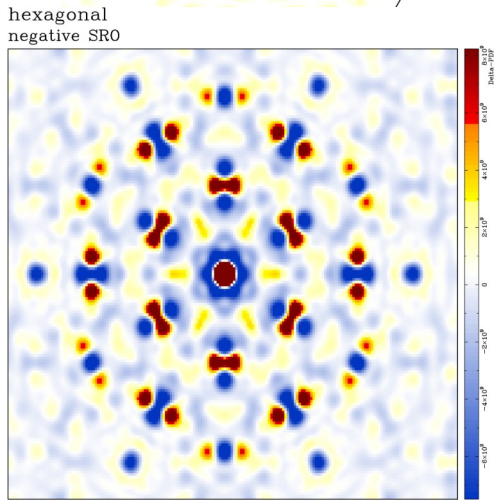
→ Hexagonal frustration!

Replace “**A**“ with **up** molecule and
“**B**” with **down** molecule



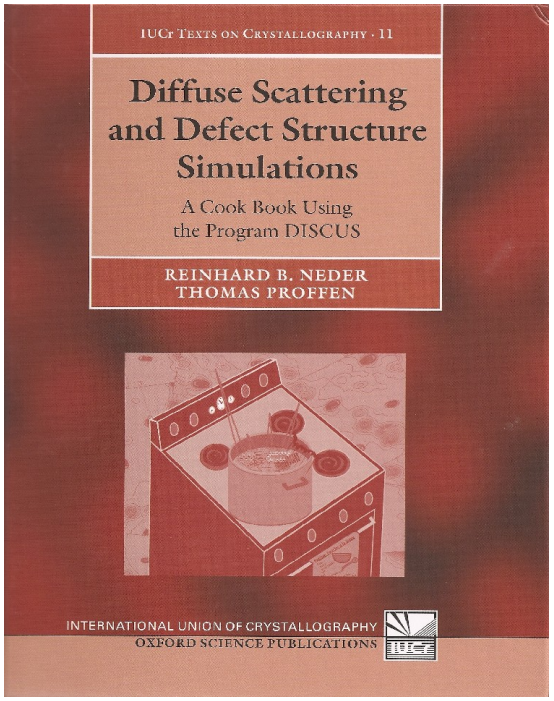






Neder, R. & Proffen, T

Diffuse Scattering and Structure Simulation, Oxford



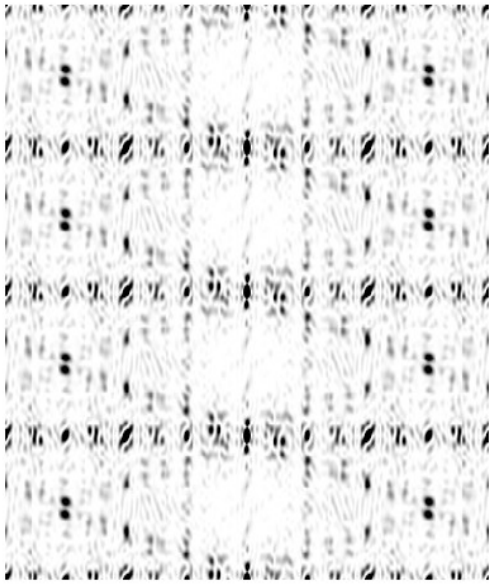
DISCUS:
www.github.com/tproffen/DiffuseCode

If you can describe it in words.
DISCUS can simulate it

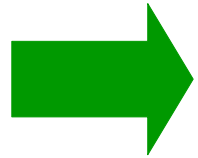
DISCUS: Workshop

Erlangen February 9 - 13
www.icsp.nat.fau.eu/neder-group/discus-home

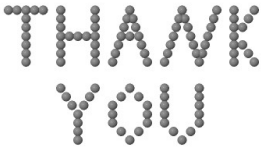
And finally



$\mathcal{F}^{-1}$



Fourier



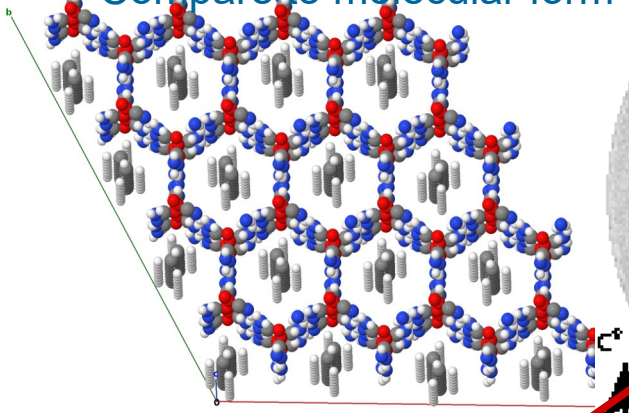
DISCUS: Workshop

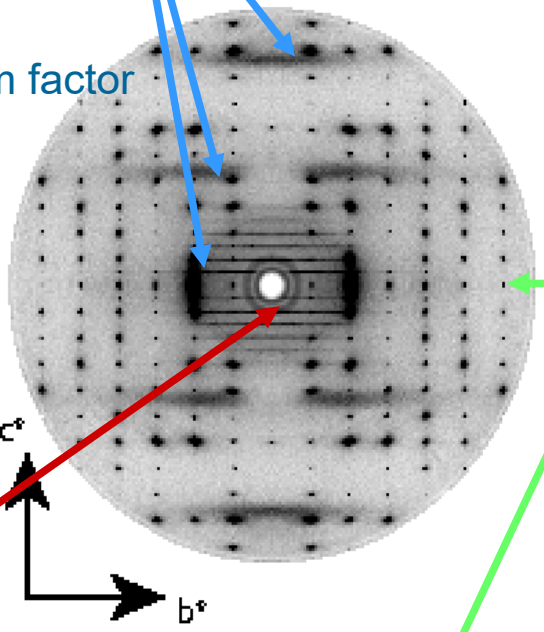
Erlangen February 9 - 13
www.icsp.nat.fau.eu/neder-group/discus-home

Very broad diffuse scattering,
no regularity in reciprocal space

→ **Scattering by single molecule ?**

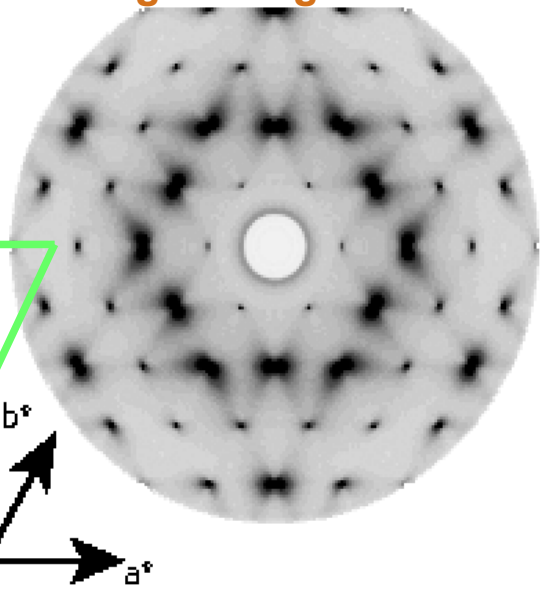
Compare to molecular form factor





Modulated diffuse scattering within planes

→ **Correlations between neighboring channels**



Sharp diffuse layers
→ **1-D disorder**

Distance between diffuse layers
→ **1-D disorder of alkane chains**

Diffuse layers fade away from reciprocal origin
→ **Predominantly substitutional disorder: Orientation in channels**

No diffuse layer at L = 0 !

$$F(hk0) = \sum f_j e^{2\pi i(hx_j + ky_j + 0z_j)}$$

Independent of z coordinates
==> hk0 *sees* projected structure

→ **No diffuse: projected structure is periodic**

Th Weber PhD München 1994

Welberry & Mayo J. Appl. Cryst 29, 1996