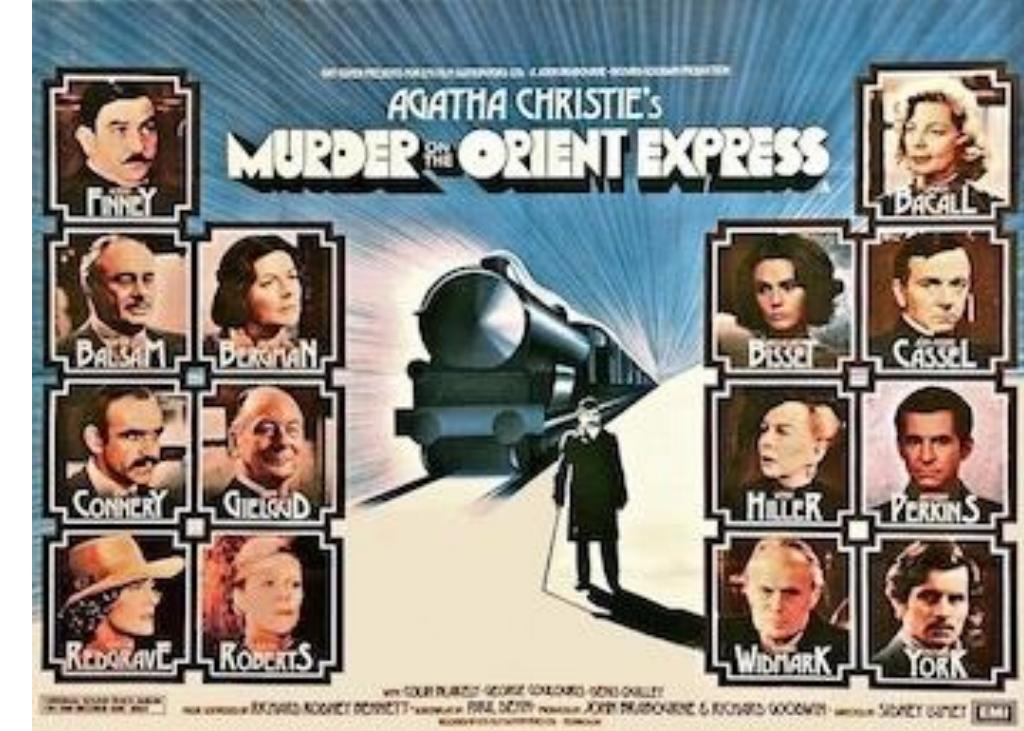
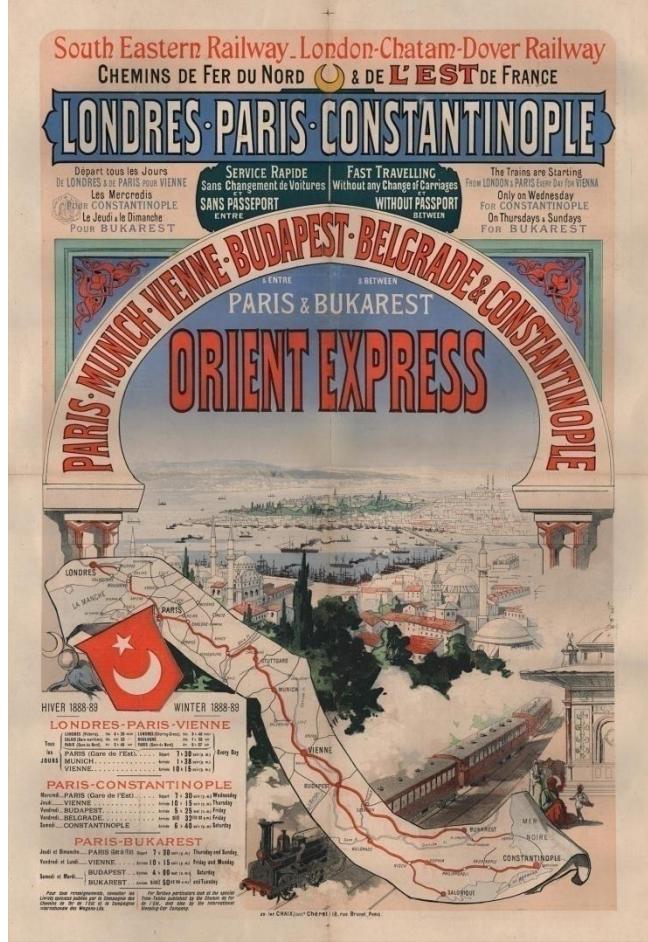
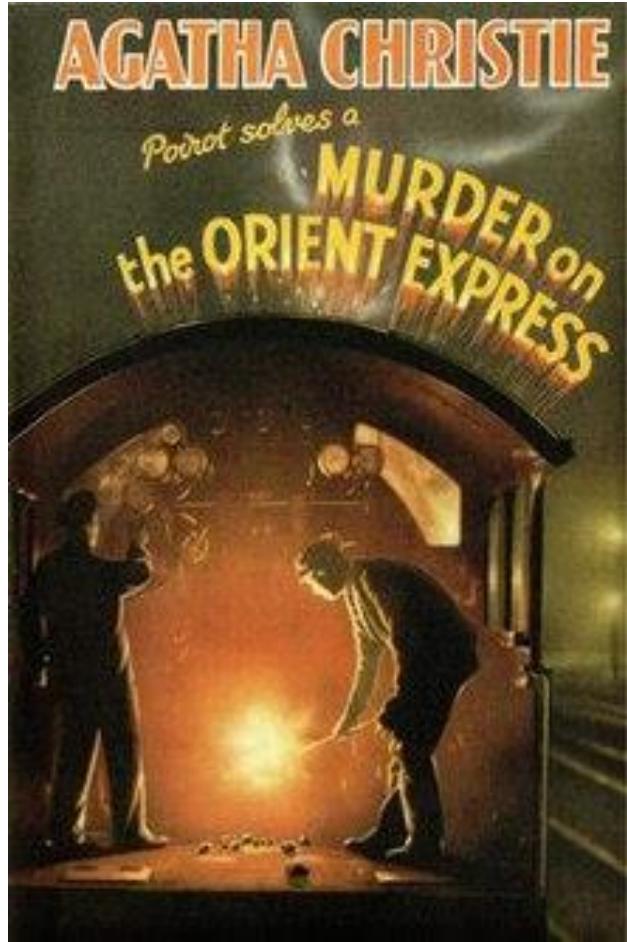


Why did those heavy fermions
gain so much weight?

*Official tour de force
de total scattering*



SCIENCE: The murder on the orient express



On my way to
the orient too

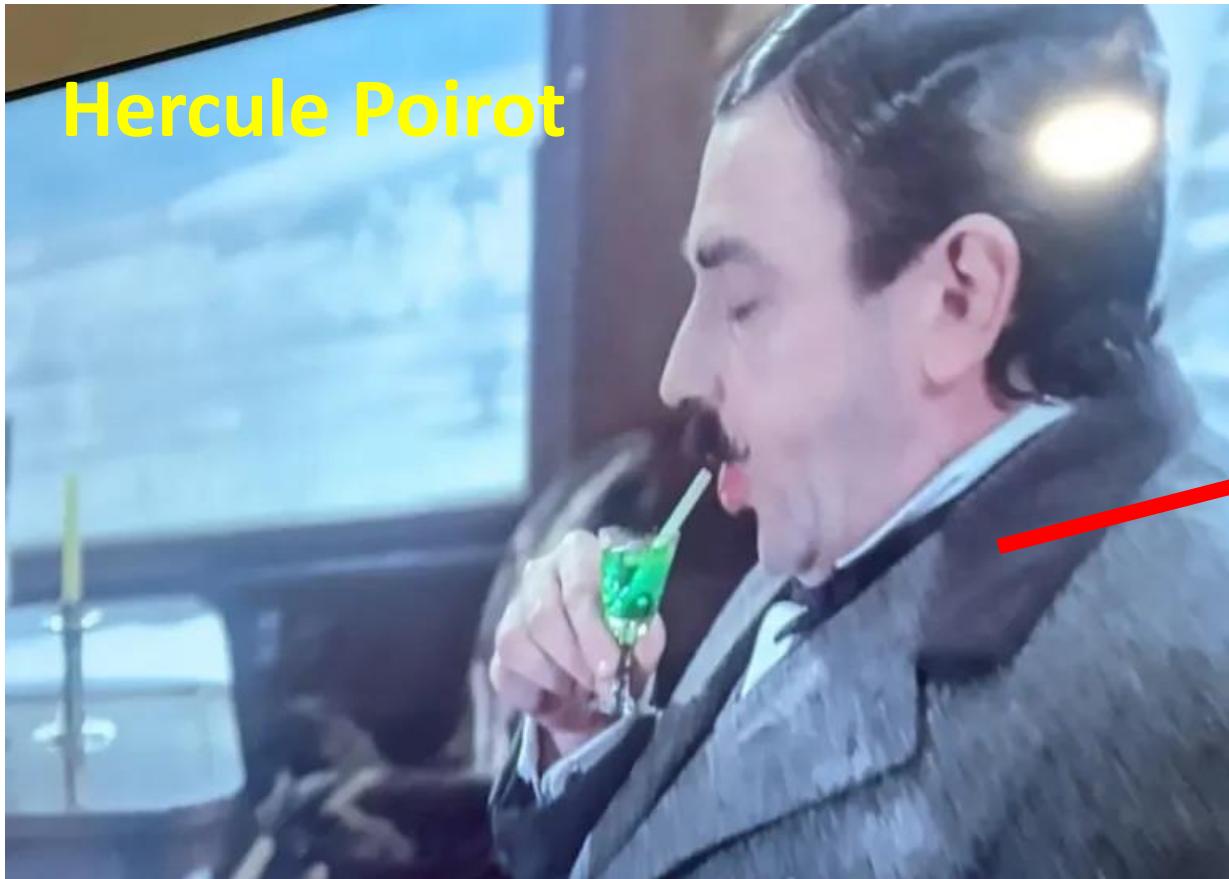


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CENTRAL MICHIGAN
UNIVERSITY



SESAME

Setting the scene.



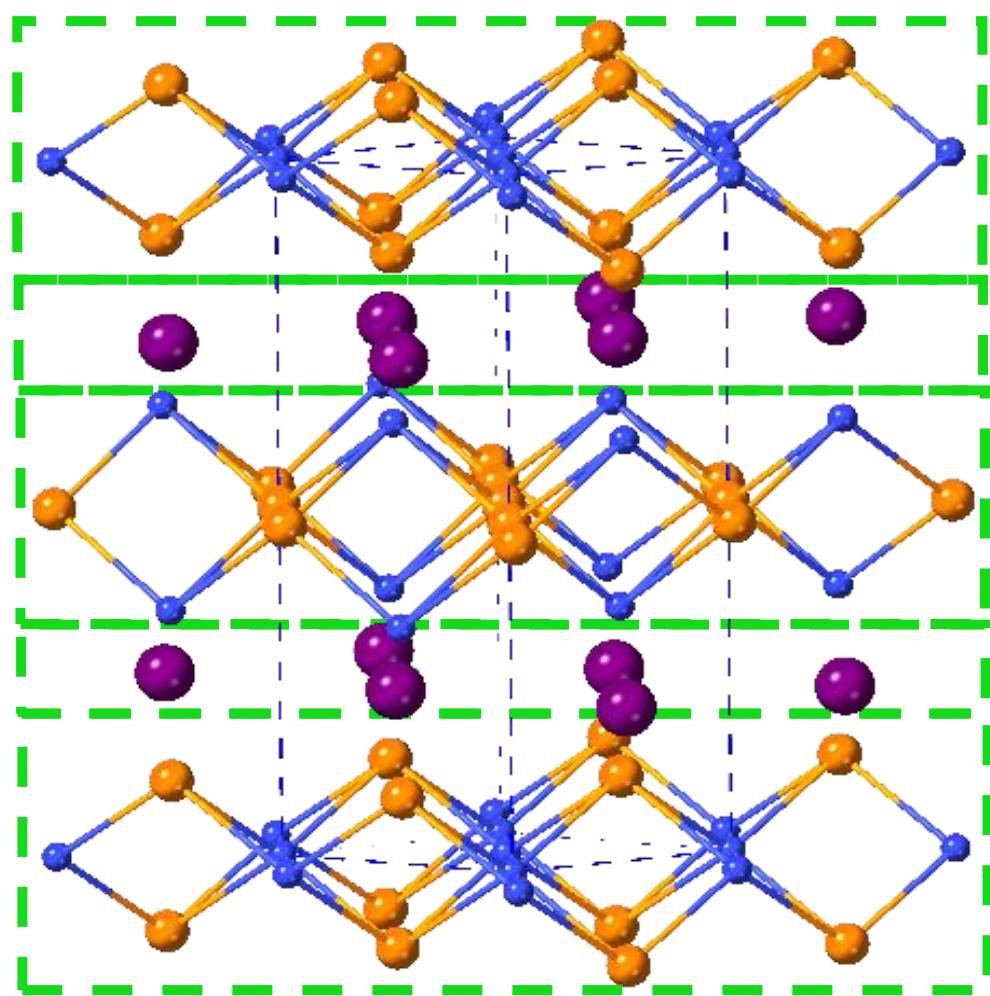
Philip Hans



Crystallography is like what we do in real life.



<https://nypost.com/wp-content/uploads/sites/2/2016/05/bear4.jpg?quality=75&strip=all&w=1024>



x
y
z



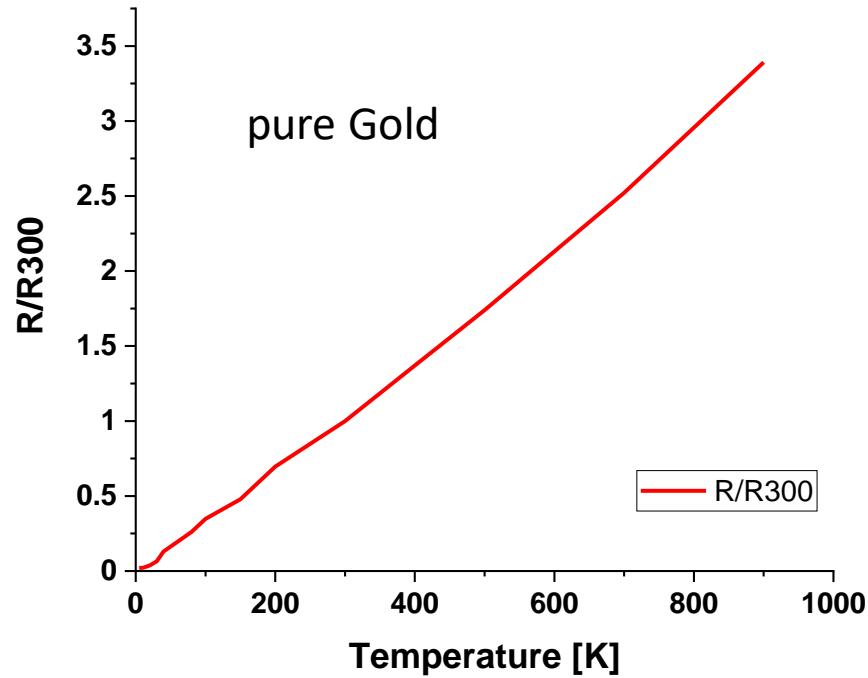
@Dells of
Wisconsin river

U ... electropositive metal
Pt ... transition metal
Si... main group element.

Superconductor?
Special magnetic
properties!

Should behave like
a metal....

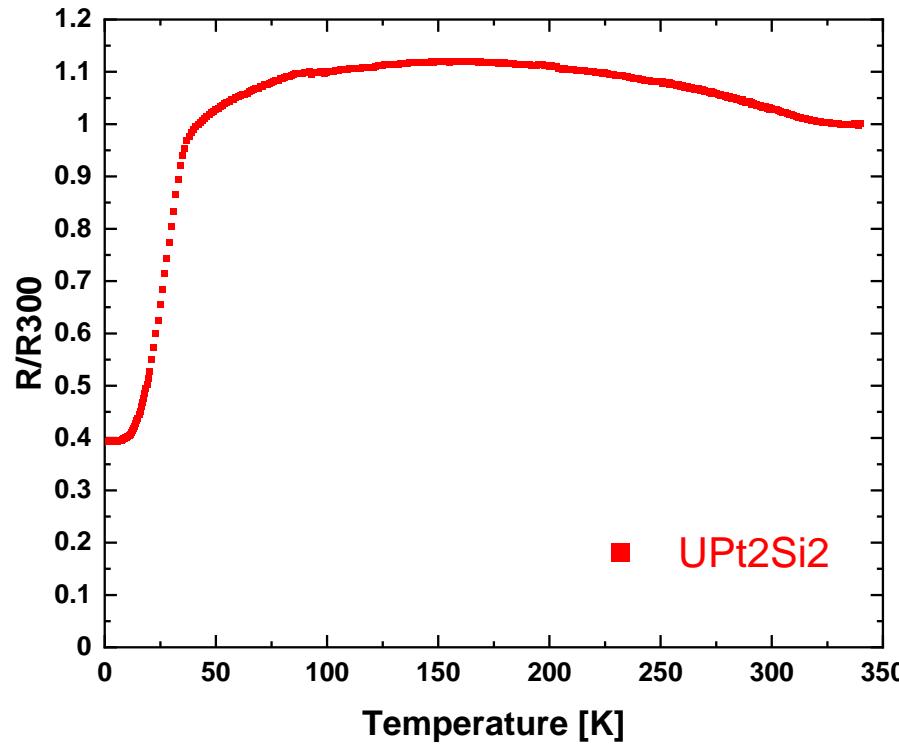
Electrical resistivity of Gold with temperature



<https://hypertextbook.com/facts/2004/JennelleBaptiste.gif>

In gold, a real metal, electrons flow
like the water in Porcupine river
- smooth and steady -

Electrical resistivity of UPt₂Si₂ with temperature

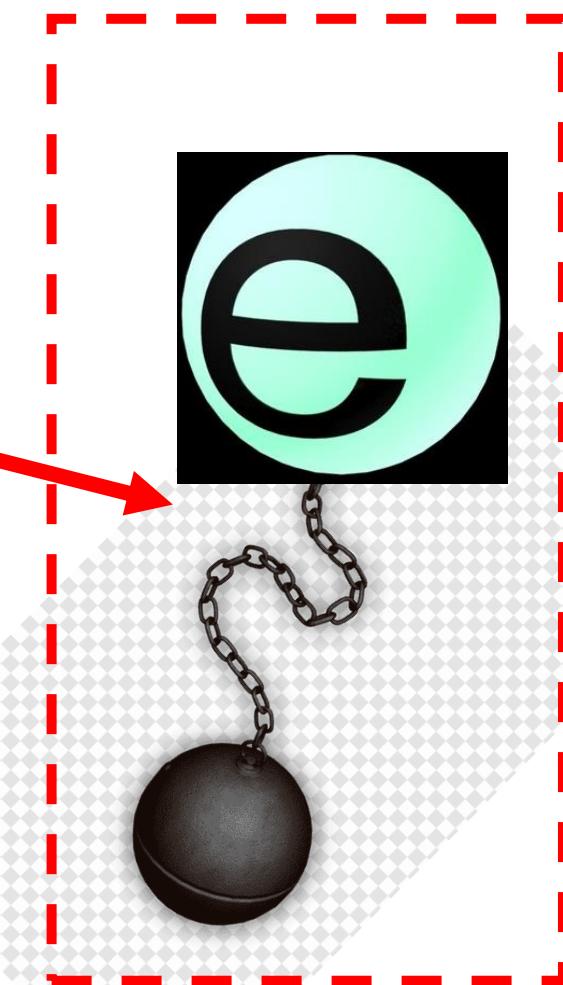


Seems as if the electrons had
troubles with getting forward.
→ Heavy electrons?

BIG QUESTION: WHY ARE THOSE ELECTRONS (FERMIIONS) SO HEAVY?



?



HEAVY FERMION



?



HYPOTHESIS

In UPt_2Si_2 , electrons become „heavy“ because they cannot move well. This is caused by the crystal structure (arrangement of atoms).

→ Let's collect some X-ray total scattering to find out more about the structure!

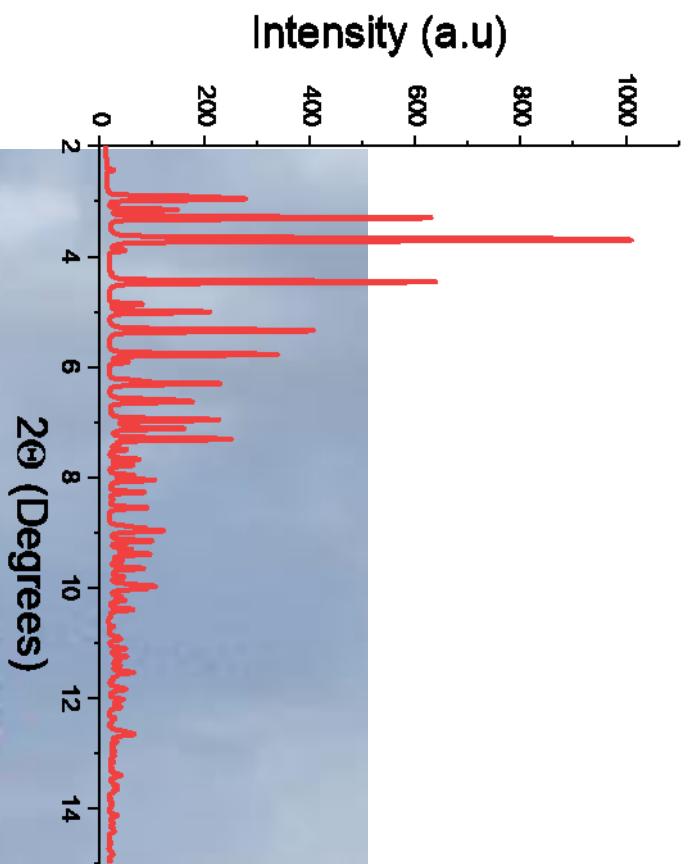


Total structure → interatomic
distances → total scattering

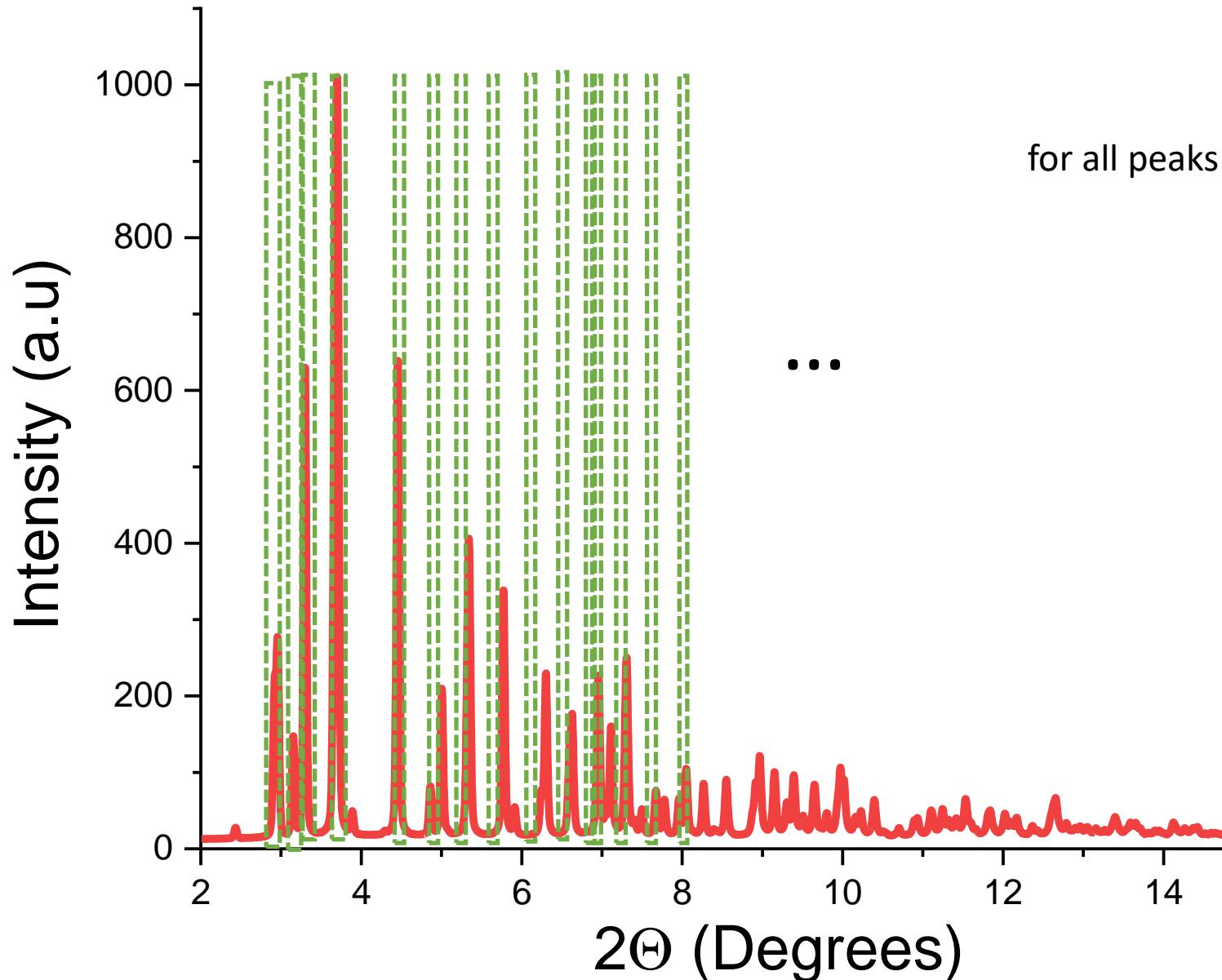


$I(Q) = \sum_i^N \sum_j^N f_i^* f_j \frac{\sin(QR)}{R}$

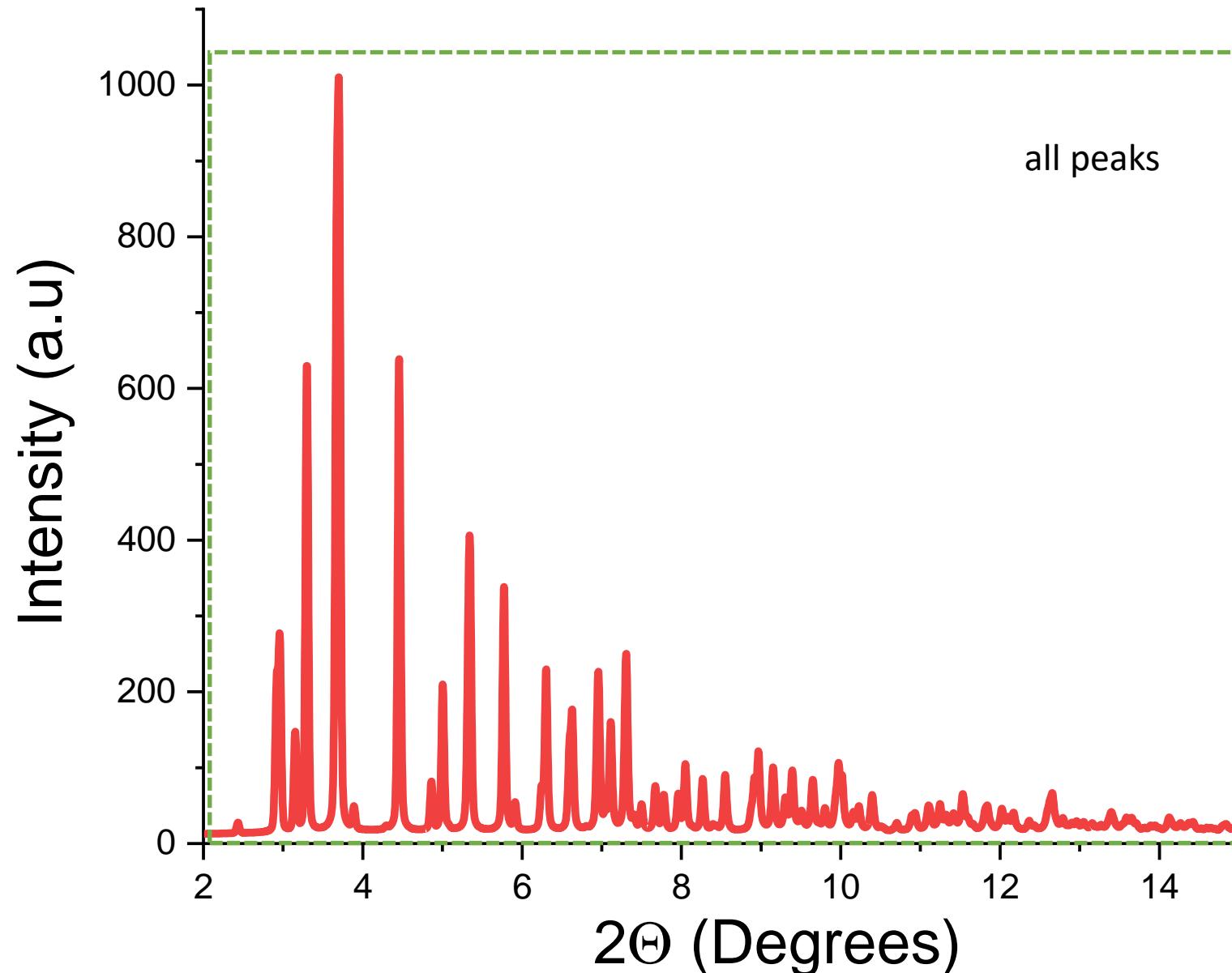
“Debye scattering equation”
Sums over all atoms
Gives total theoretical intensity



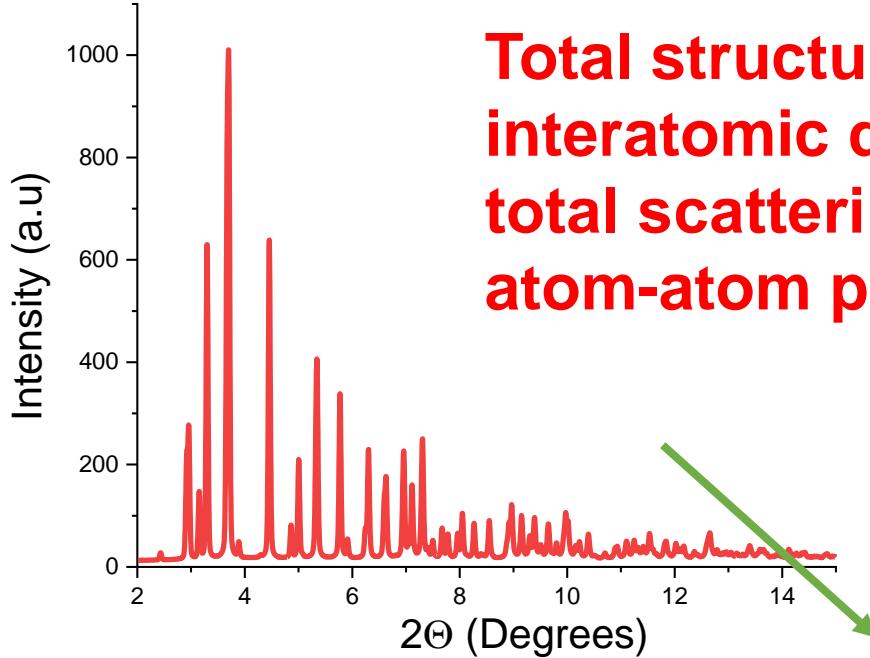
„CONVENTIONAL ANALYSIS“ OF DIFFRACTION DATA



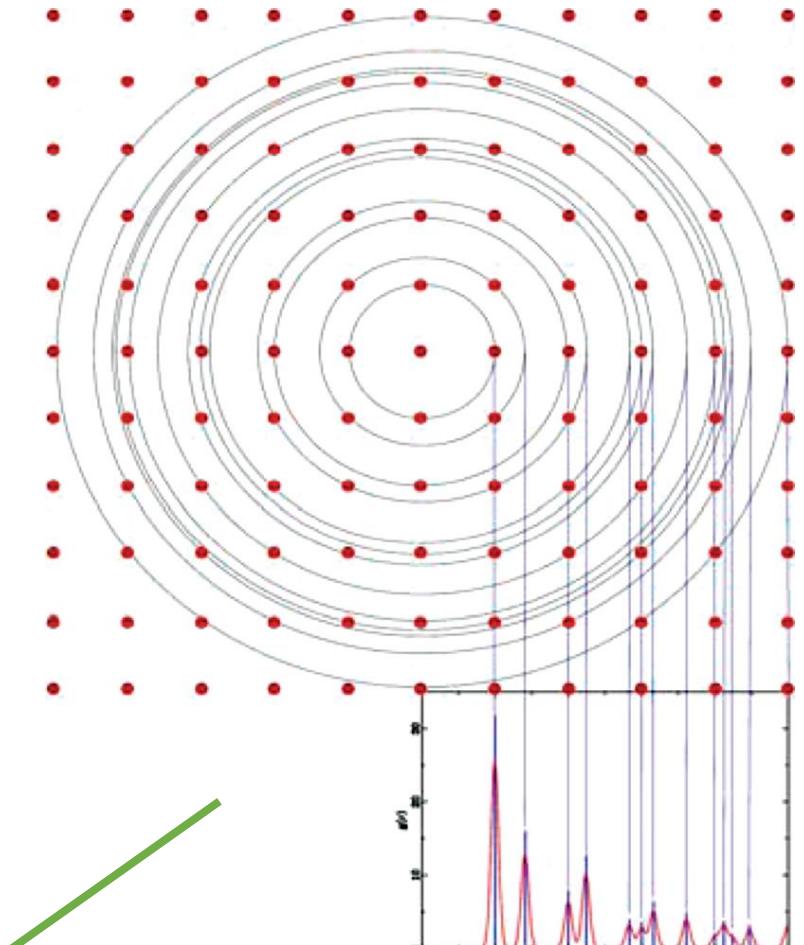
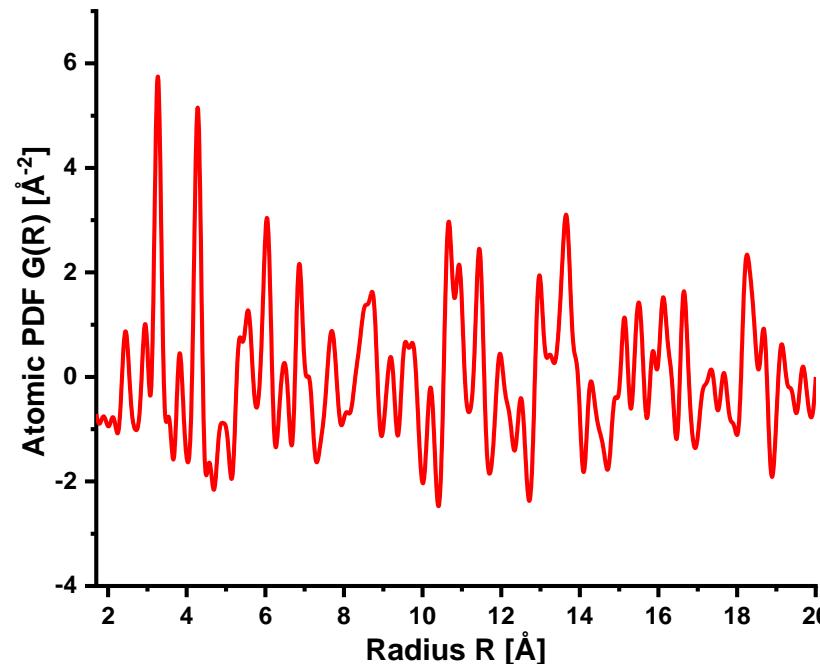
TOTAL SCATTERING APPROACH



Total structure →
interatomic distances →
total scattering →
atom-atom pair distribution function

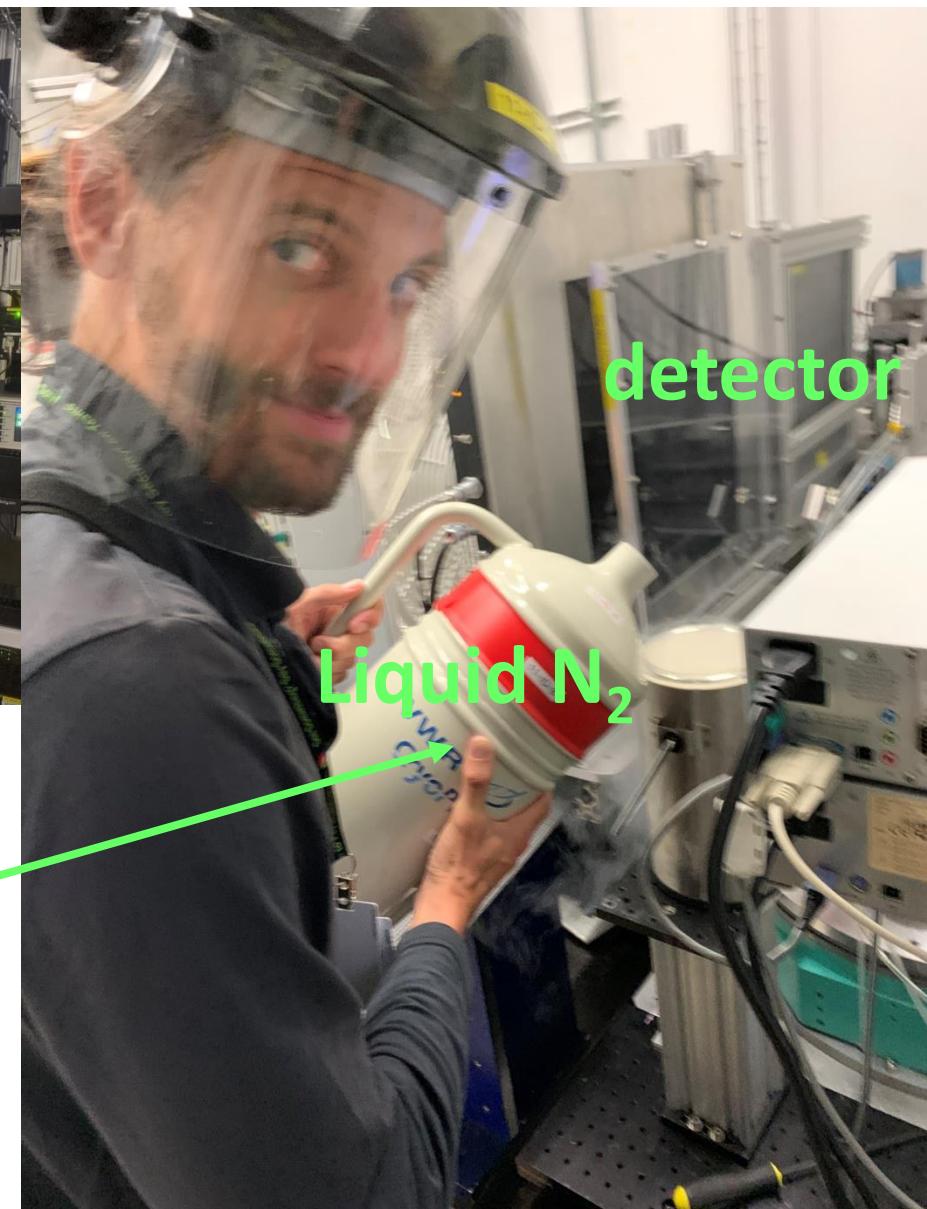
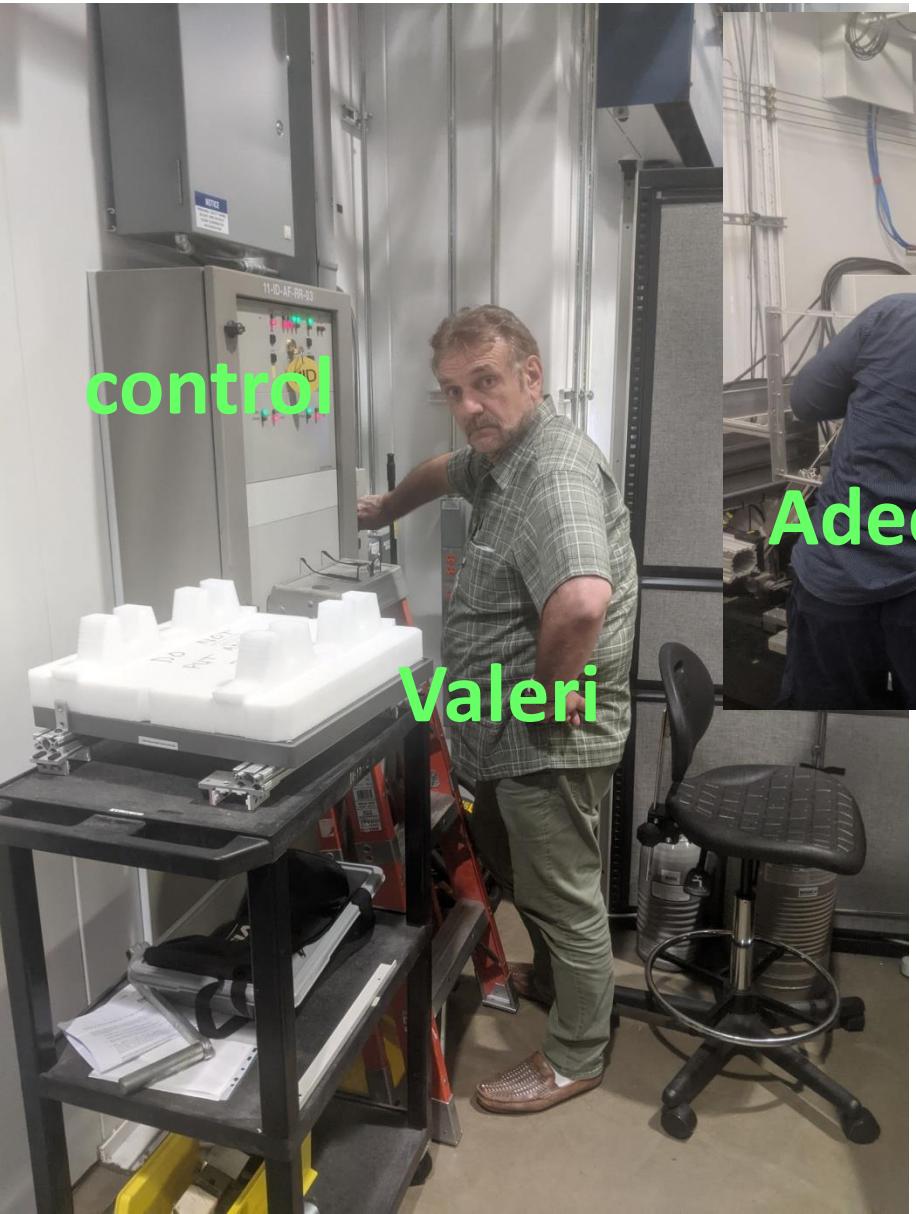


Corrections,
approximations,
Normalizations,
Mathematical transformation of
representation of information



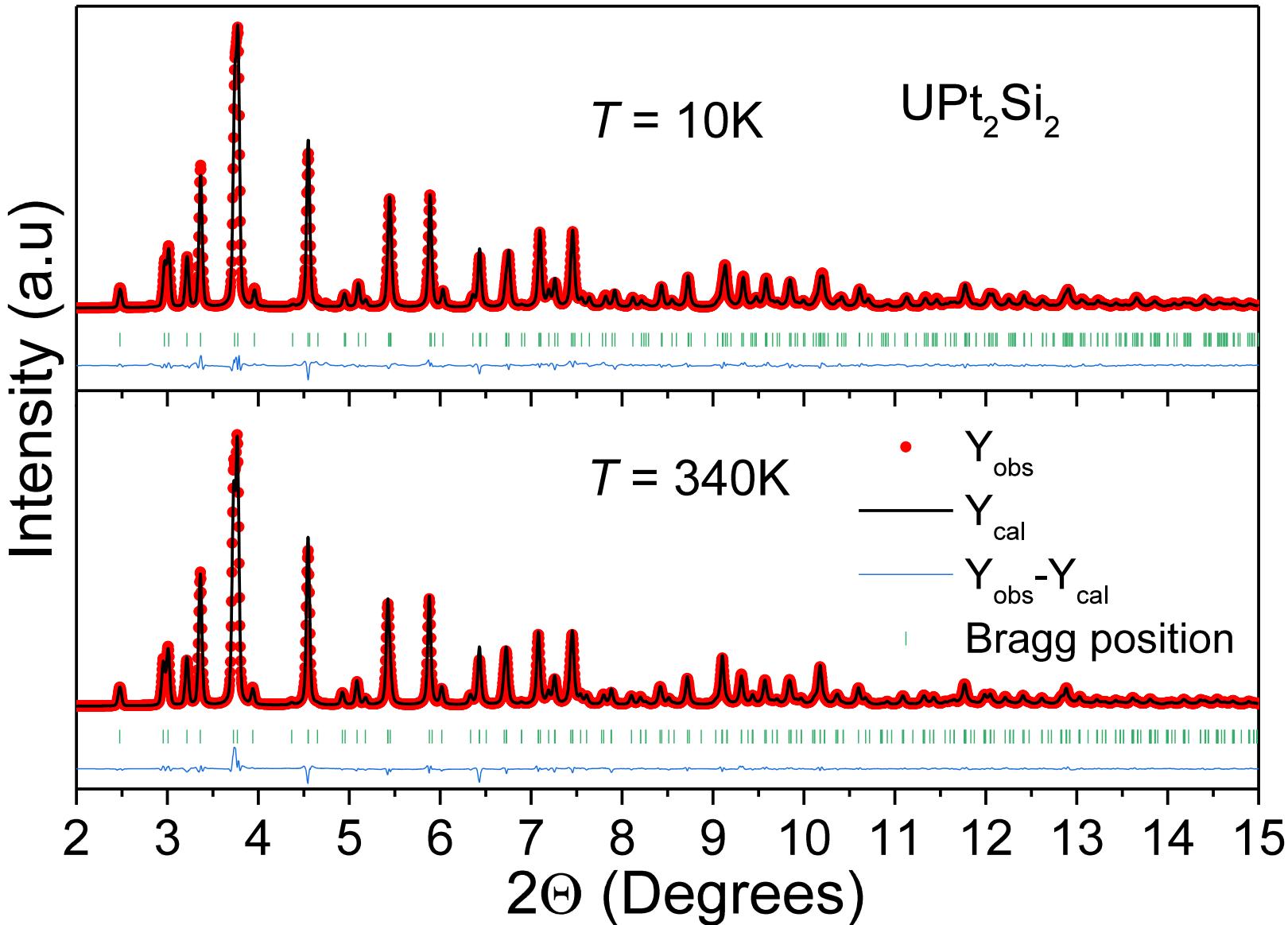
Petkov (2012) - PAIR DISTRIBUTION FUNCTIONS ANALYSIS

ACTION: Let's collect some X-ray total scattering

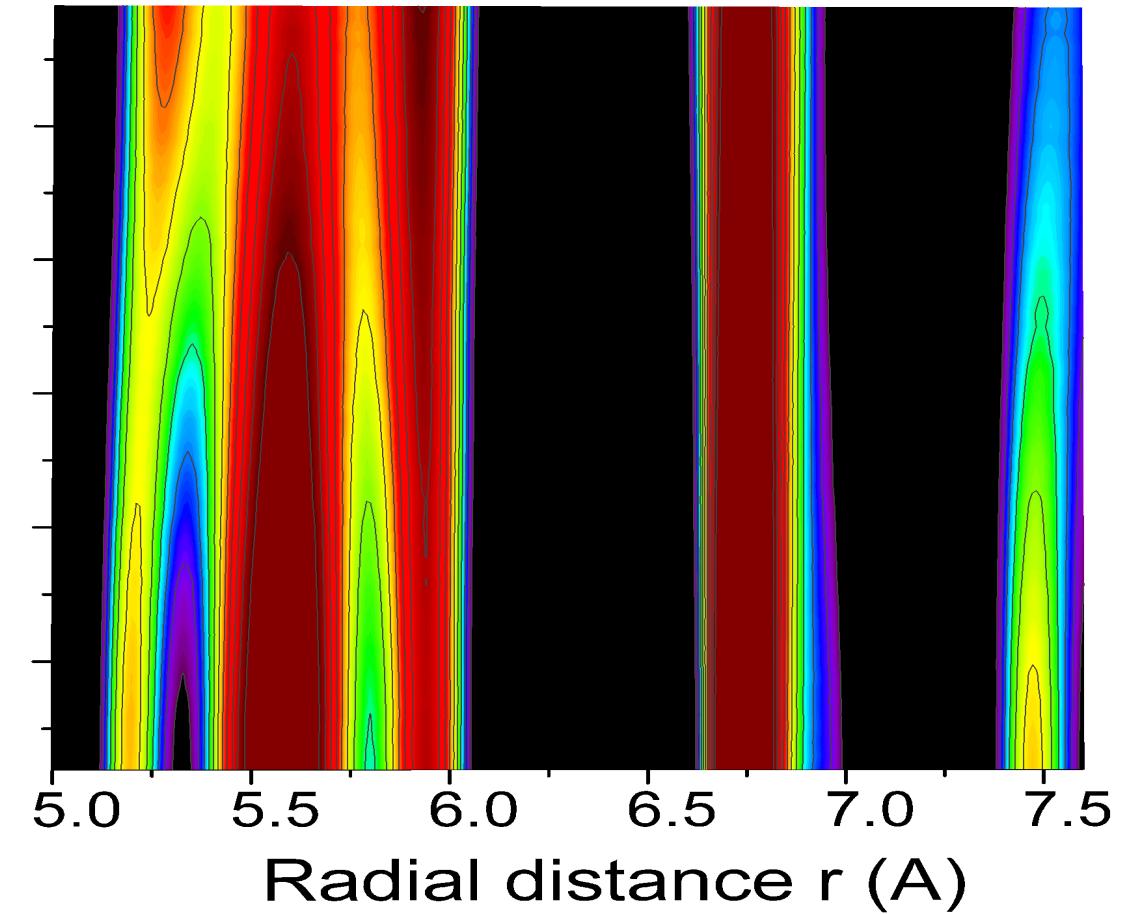
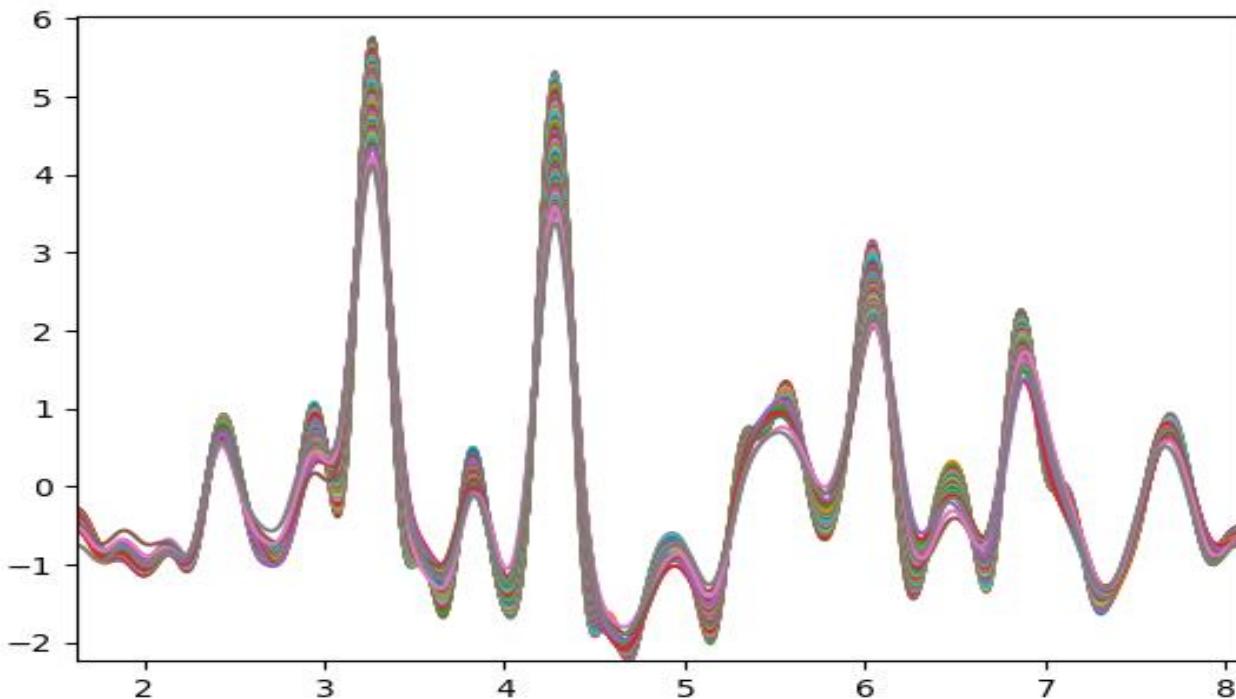


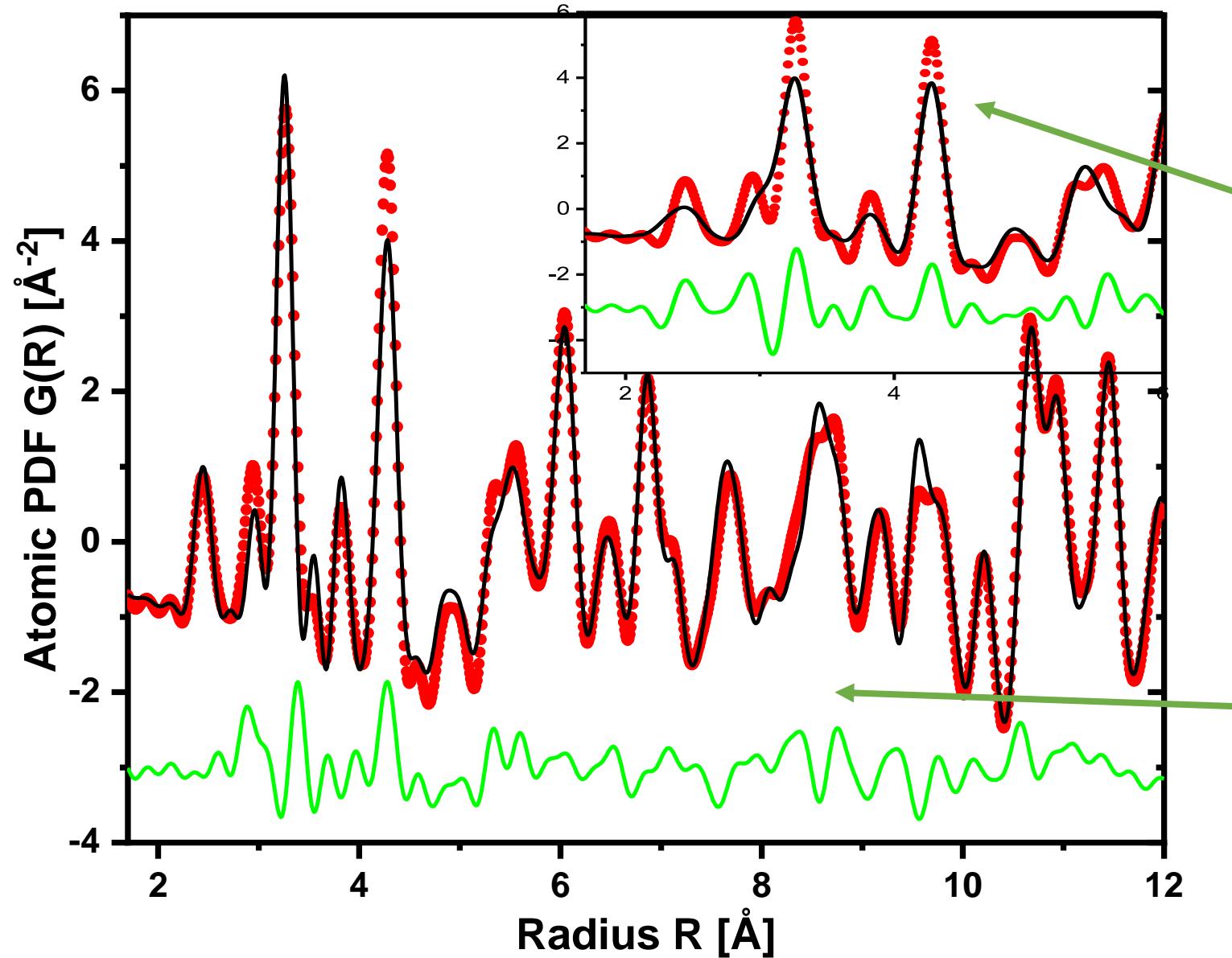
Conventional structure analysis (Rietveld)

-> structure shows spacegroup P4/nmm at all T



But PDF from powder XRD data show evolution with temperature, so the structures changes.





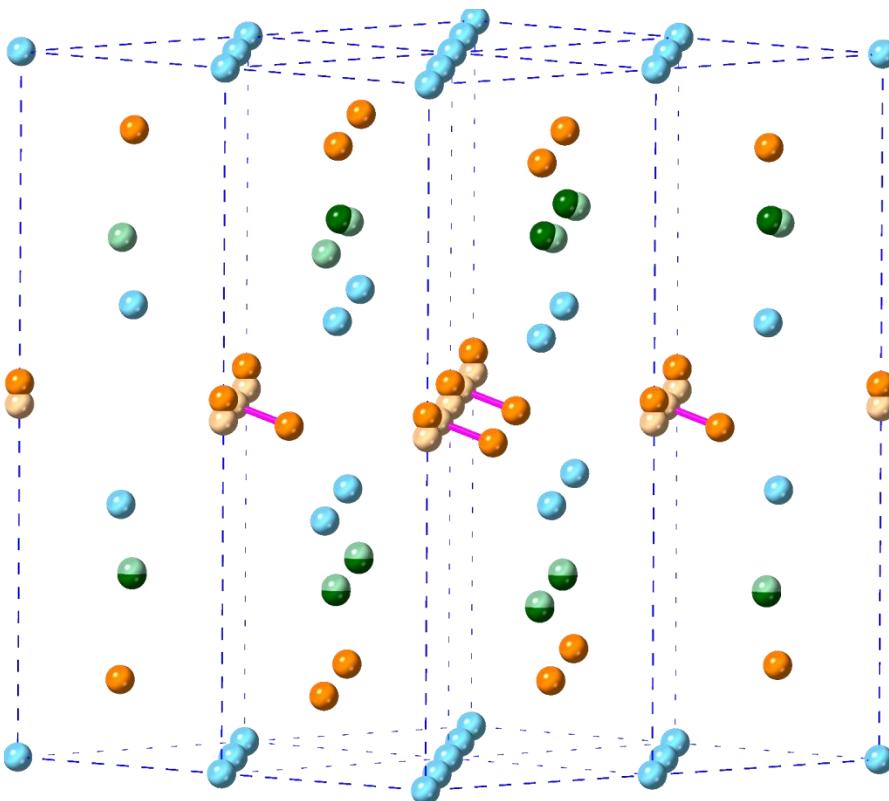
Model from
Rietveld refinement

Model from
PDF refinement

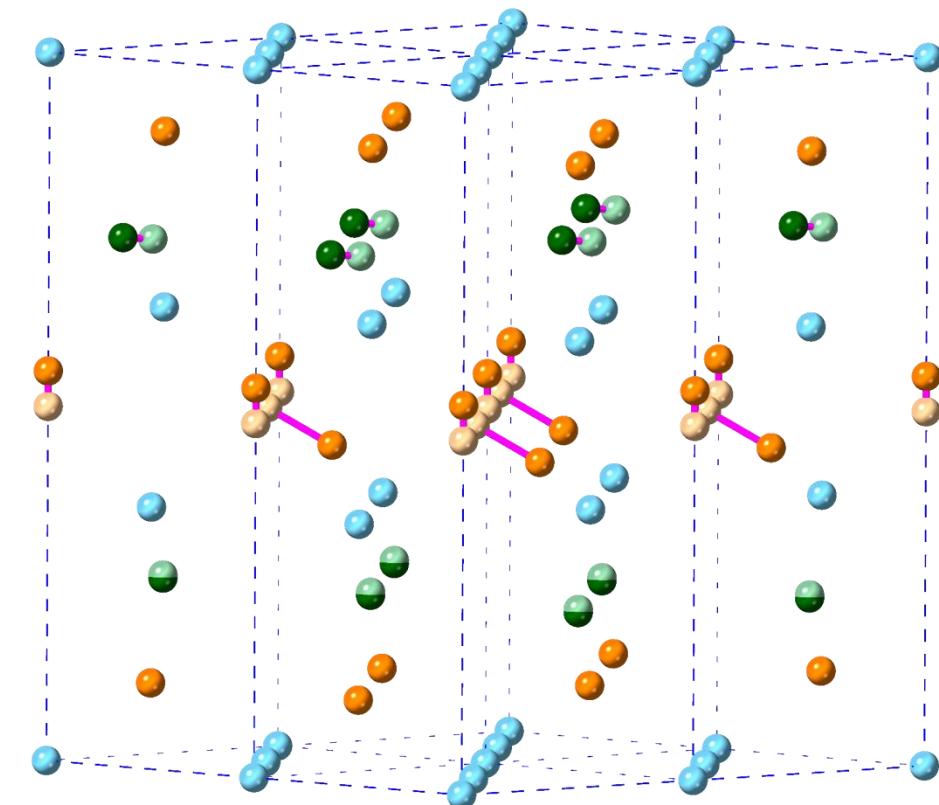
PDF from total scattering reveals deviation from average structure.

Small box PDF-refinements: UPt_2Si_2

UPt_2Si_2 350K

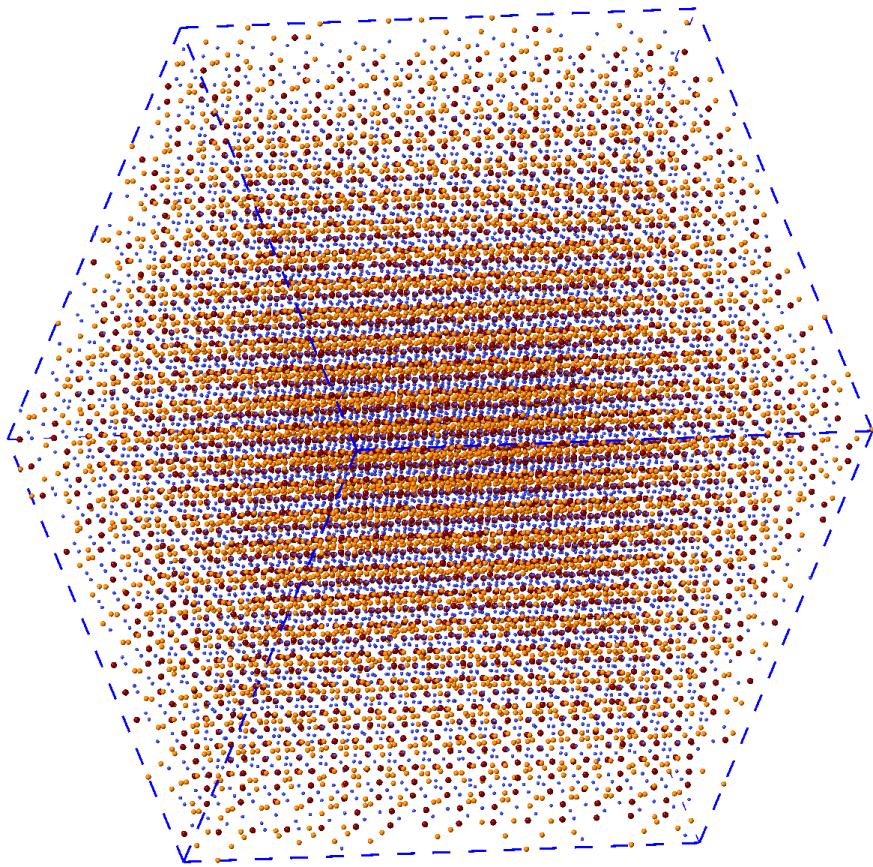


UPt_2Si_2 10K



Is there disorder?

Reverse Monte Carlo refinements for UPt_2Si_2



15x15x7
15750-atoms supercell

- Parameter space: the positions of atoms of the material under study put in a 'box', with the required density

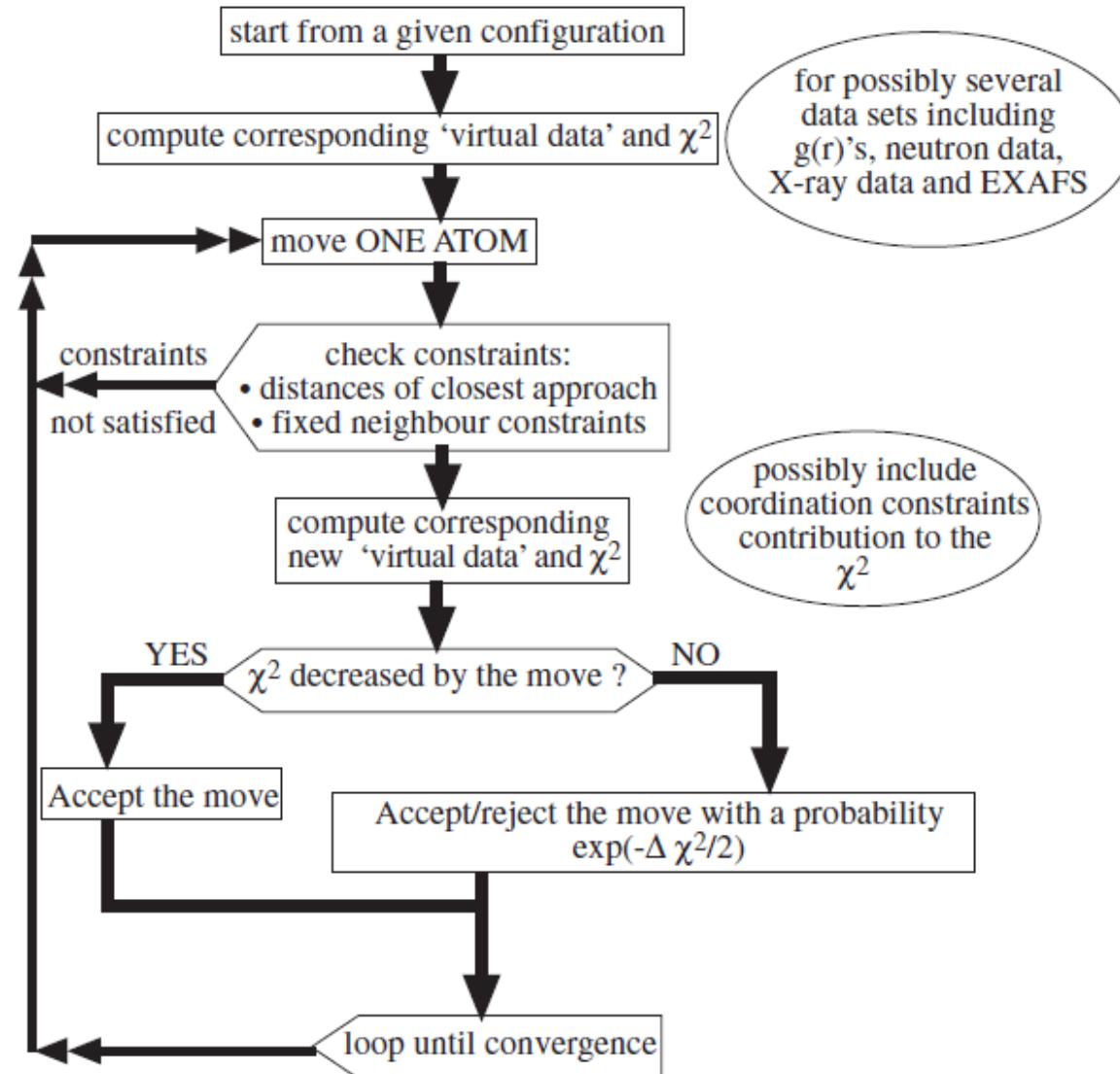
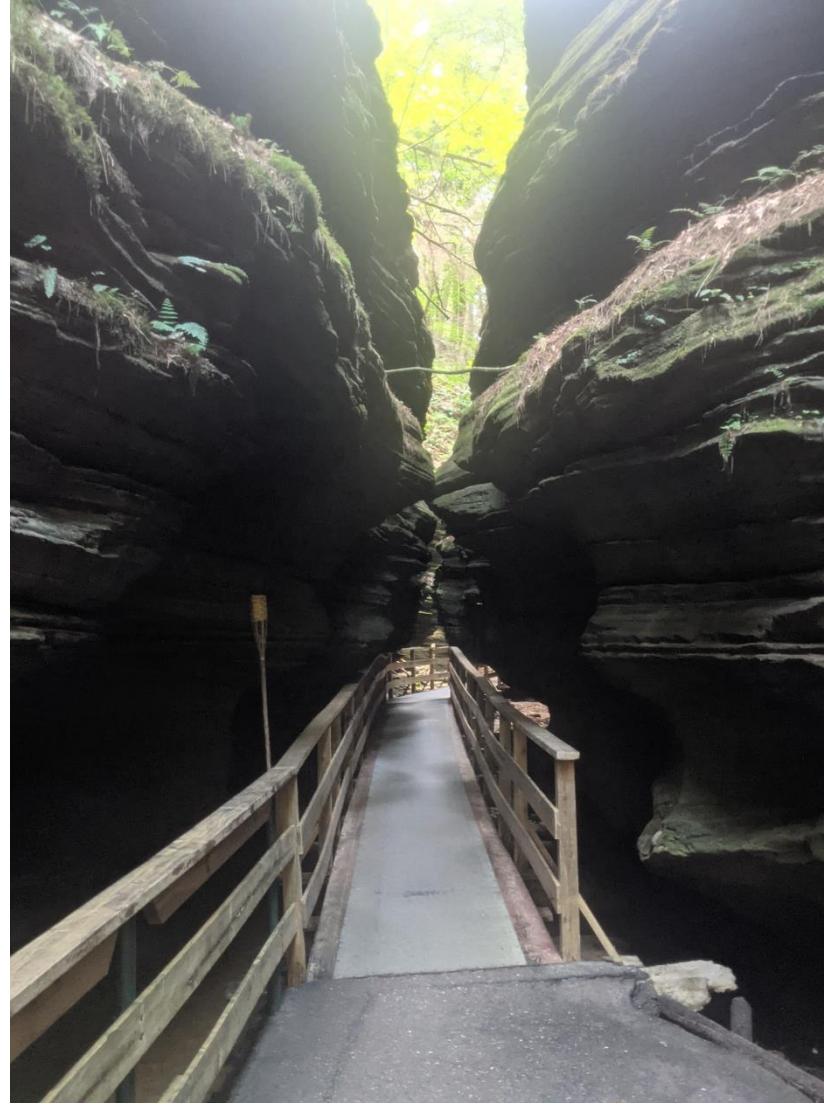
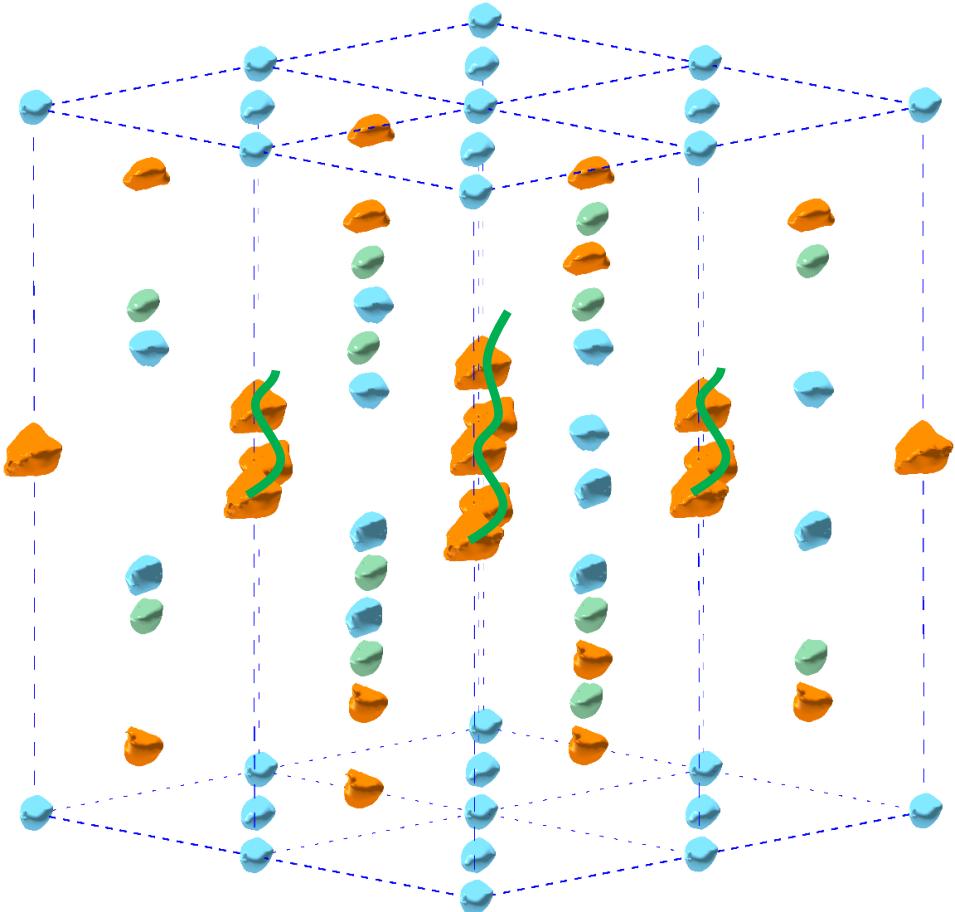
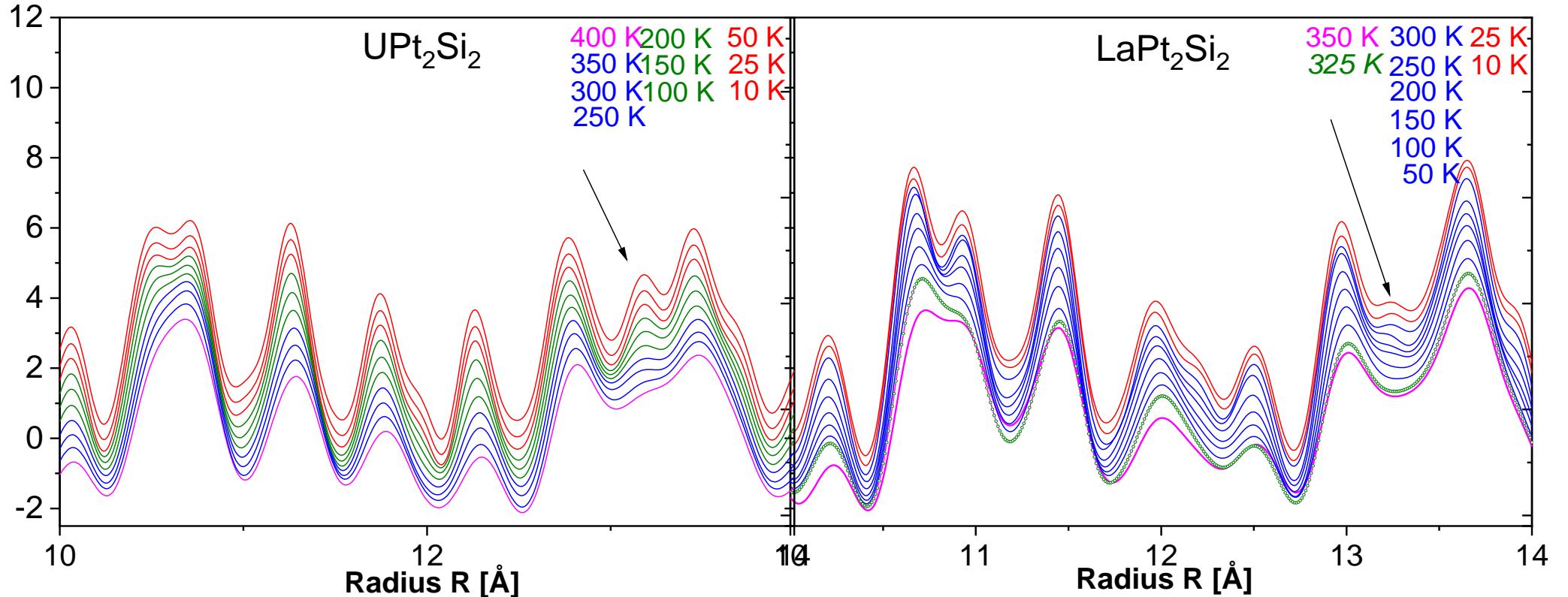


Figure 2. Flowchart of the 'standard' RMC algorithm.

RMC – 15x15x7 collapsed to 1x1x1 unit cell (10K)



Moreover:
New distances are already visible without modelling.



Comparison of isostructural (really???)
 UPt_2Si_2 and LaPt_2Si_2 .

PDF: we can already see that something happens without explanation



more bang for the buck! - If YOU want to discuss, shoot me a line!

phlpp.hns@gmail.com

