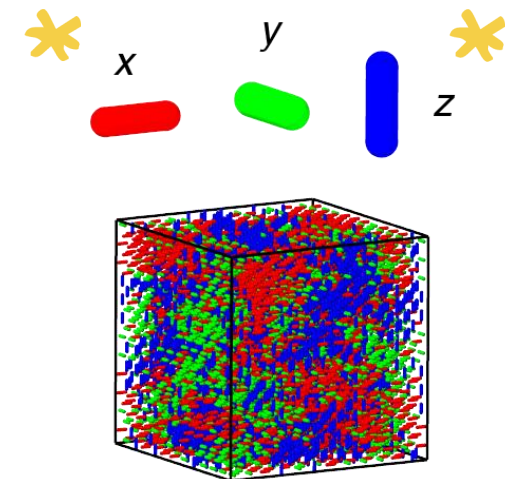
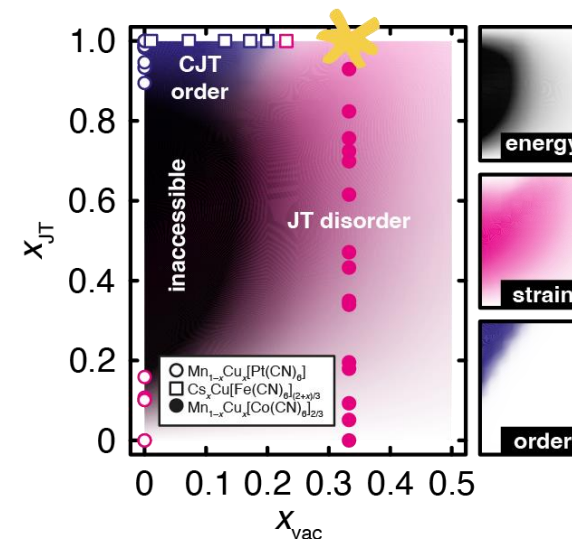
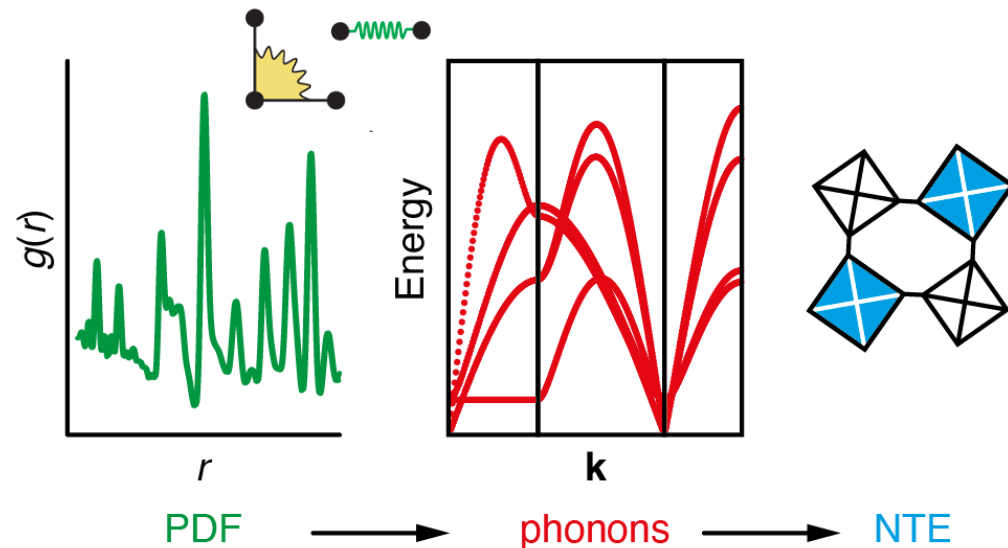
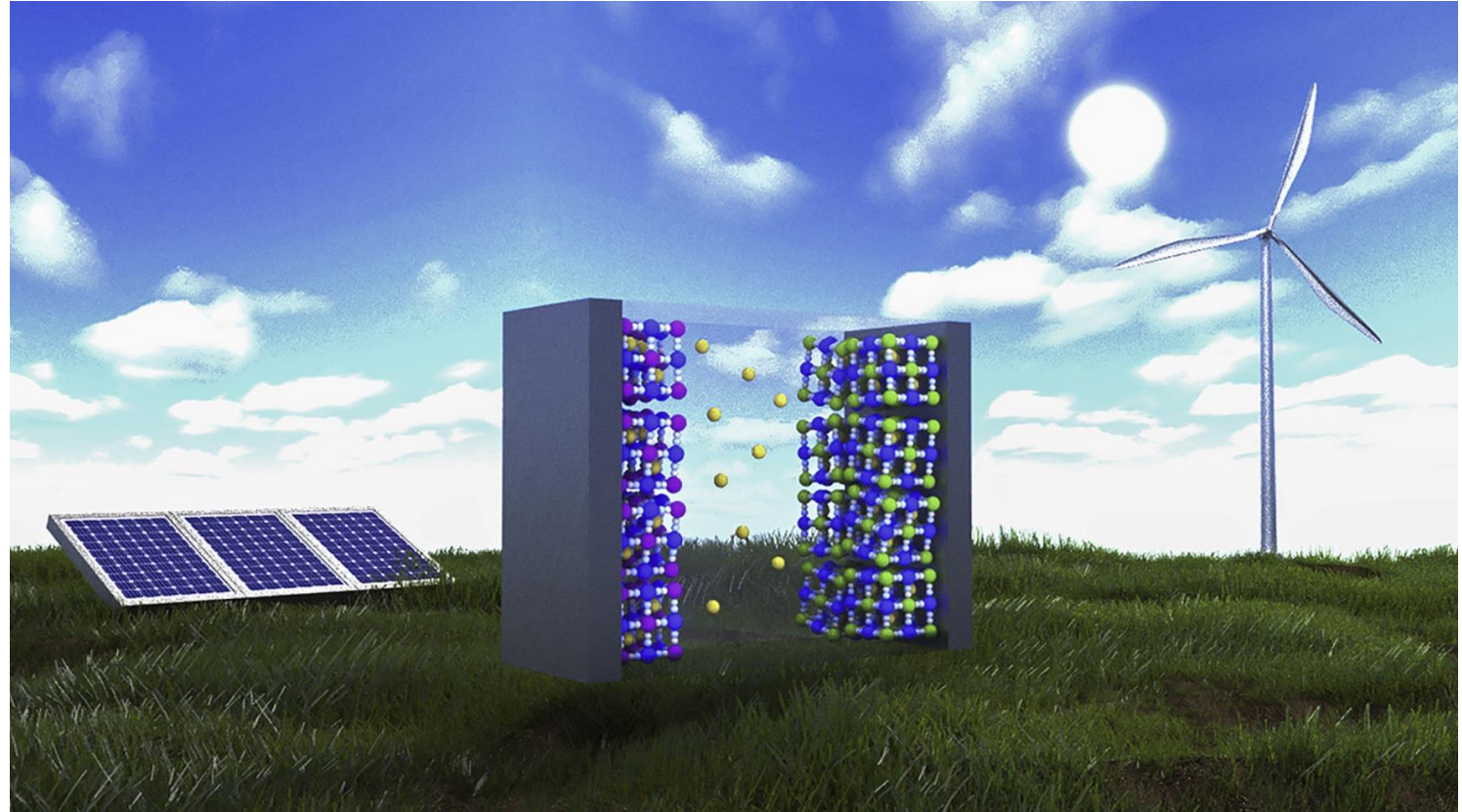


Understanding local structure and dynamics in Prussian blue analogues

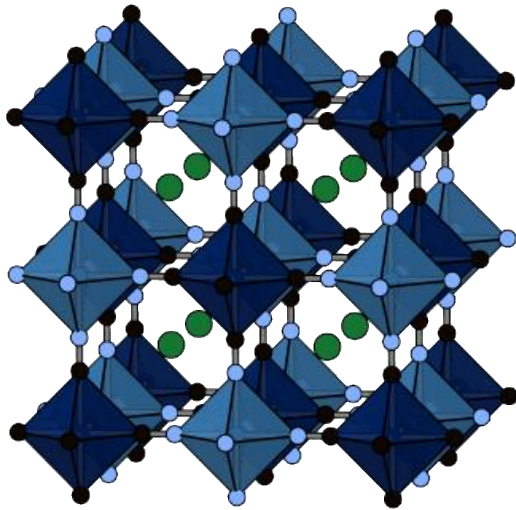
Elodie A. Harbourne, David A. Keen, Andrew L. Goodwin



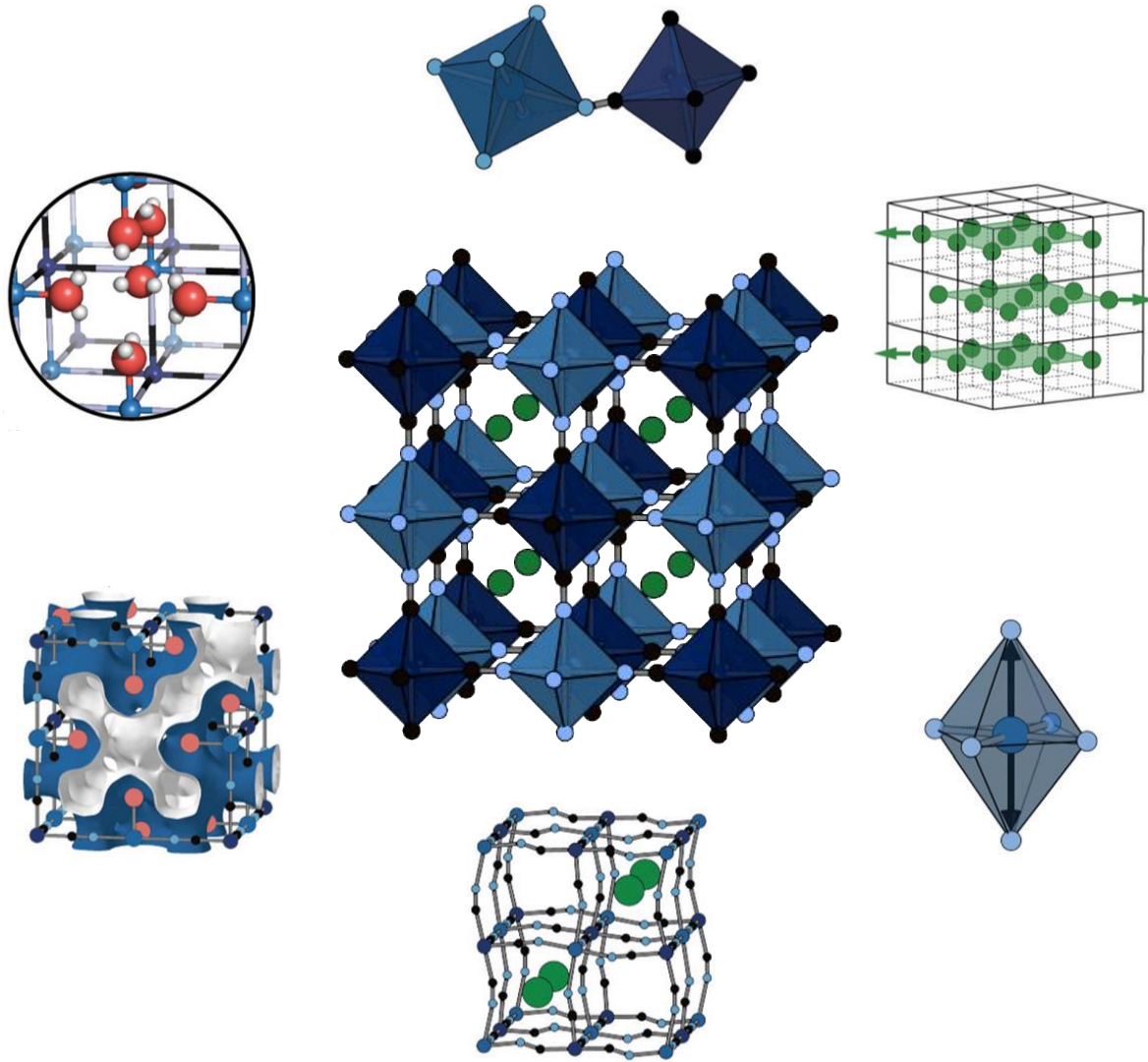
Prussian blue analogues (PBAs) - Background



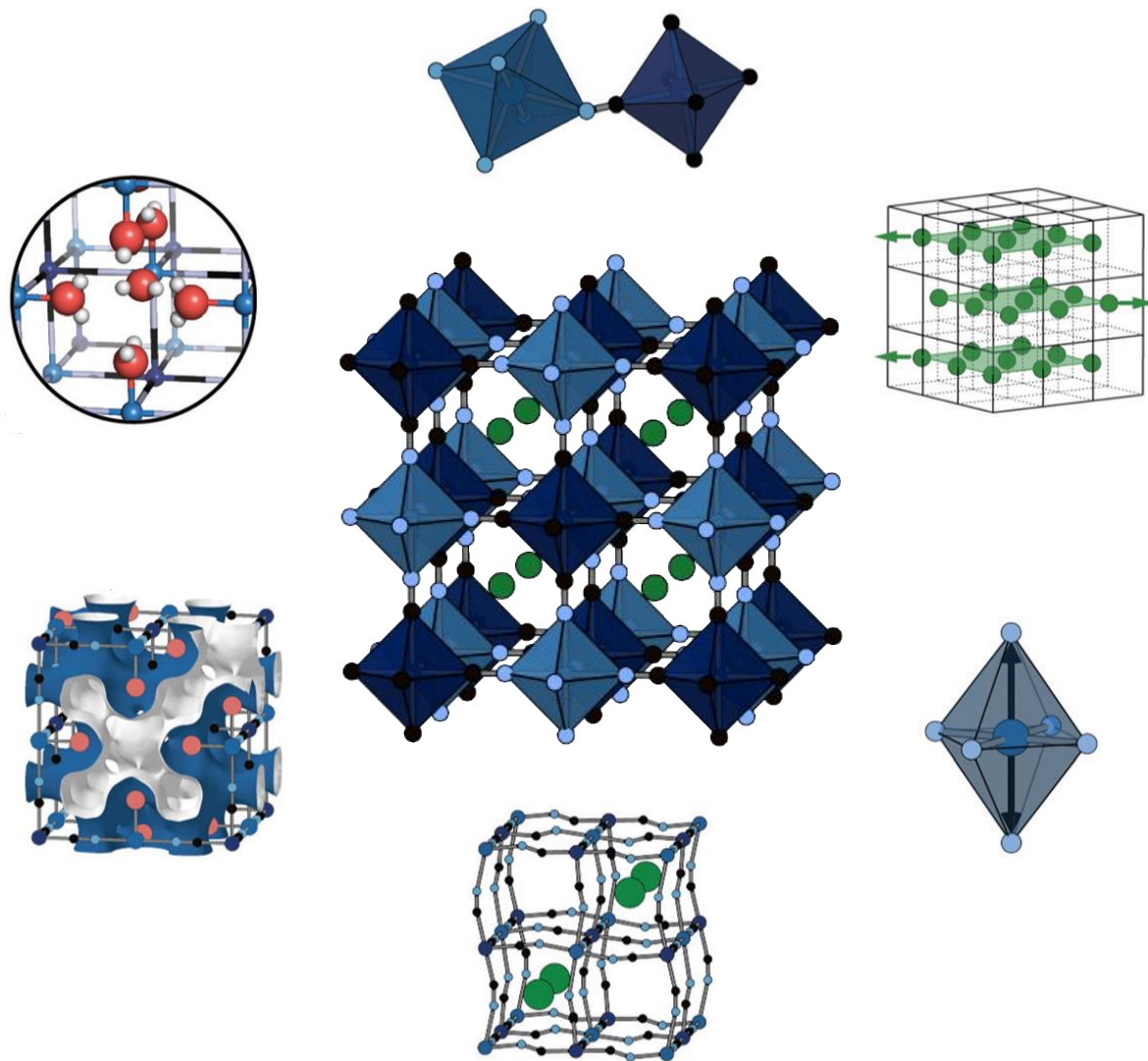
Structural complexity in PBAs



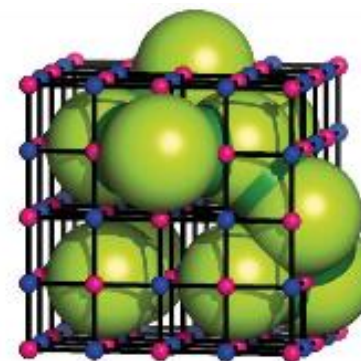
Structural complexity in PBAs



Structural complexity in PBAs

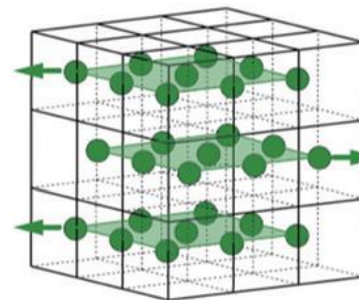


J. Cattermull, M. Pasta, A. L. Goodwin, *Mater. Horiz.*, **2021**, 8, 3178



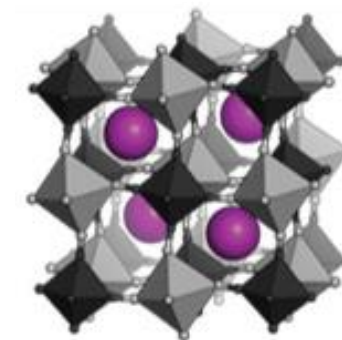
Correlated vacancies

Simonov *et al*,
Nature **2020**,
578, 256



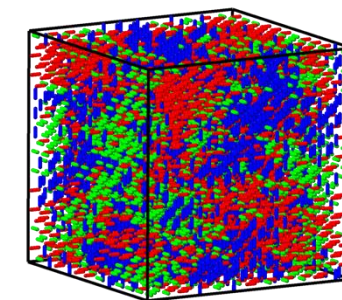
A-site 'slides'

Cattermull *et al*,
JACS **2023**, 145,
24249



Octahedral tilts

Boström & Brant,
J. Mater. Chem. C.
2022, 10, 13690

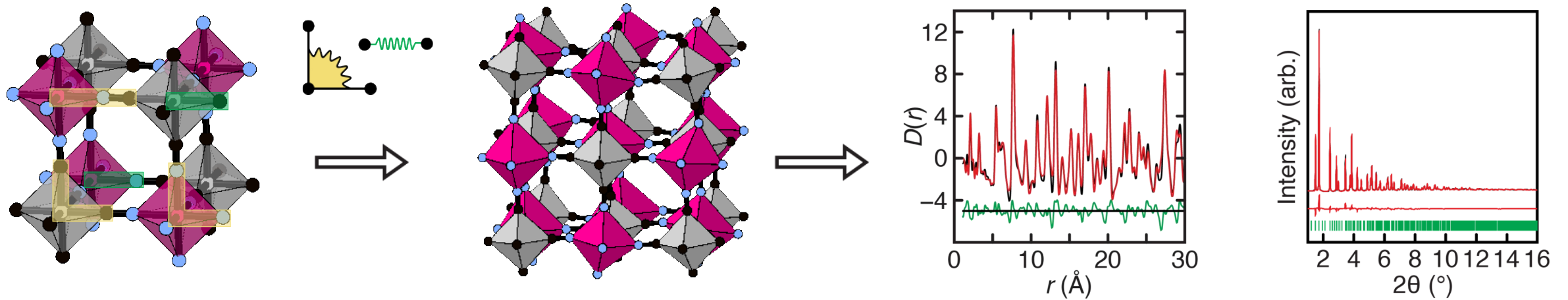


Cooperative JT

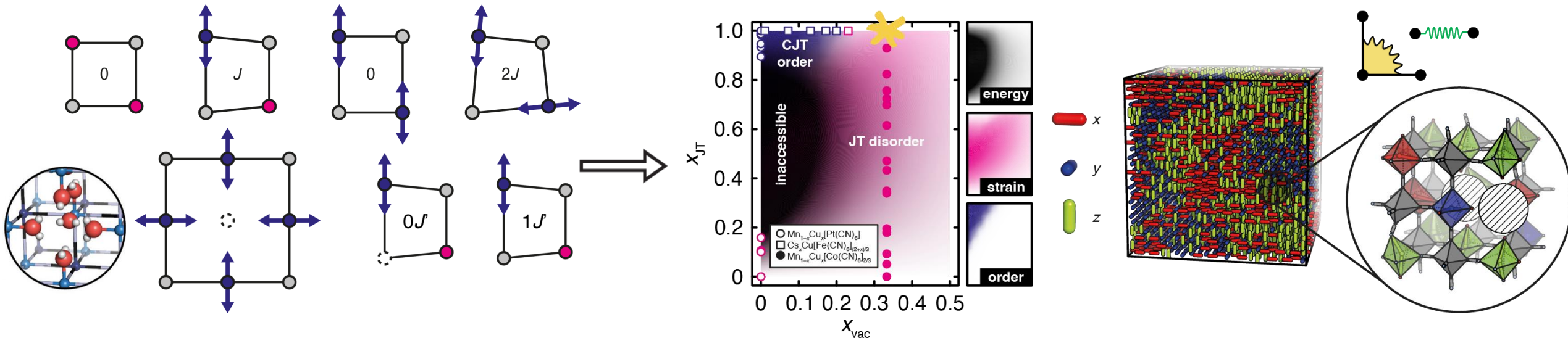
Harbourne *et al*
arXiv:2408.13169
2024

Talk overview

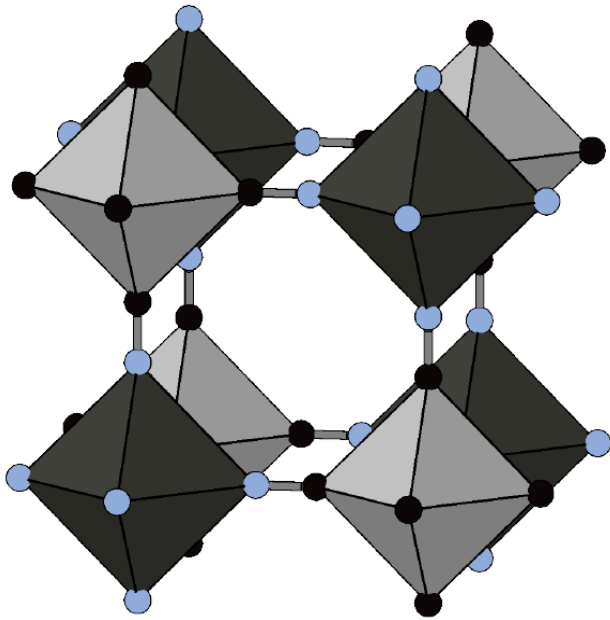
1. 'Interaction-space' Monte Carlo-driven big-box modelling of 'simple' PBAs



2. Rules governing Jahn–Teller order in PBAs and the interplay of JT/vacancies



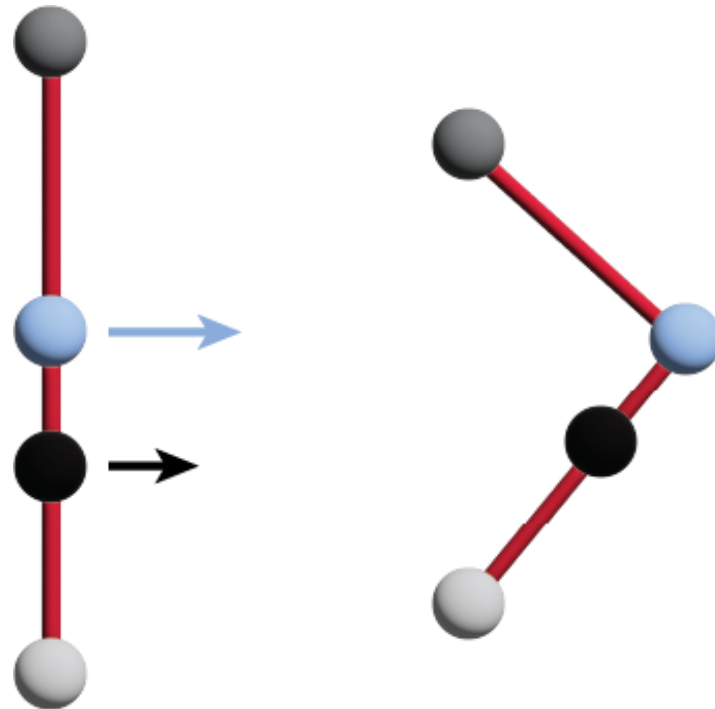
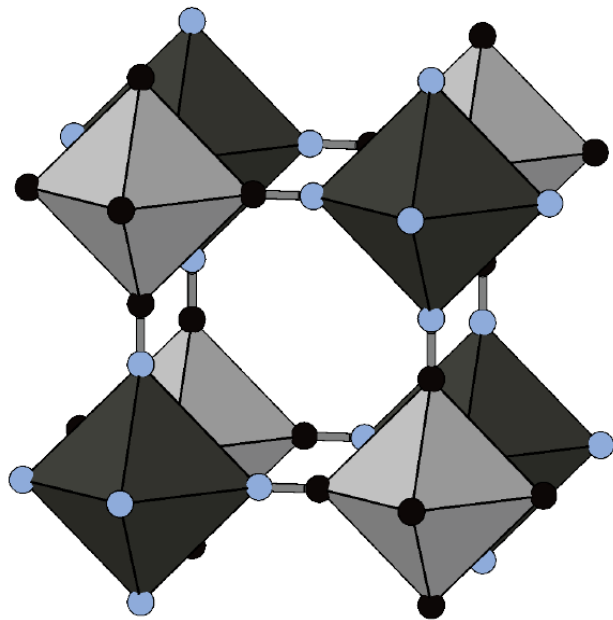
Negative Thermal Expansion (NTE) in $\text{MPt}(\text{CN})_6$ PBAs



A. L. Goodwin, K. W. Chapman, C. J. Kepert, *J. Am. Chem. Soc.*, 2005, 127, 17980

K. W. Chapman, P. J. Chupas, C. J. Kepert, *J. Am. Chem. Soc.*, 2006, 128, 7009—7014

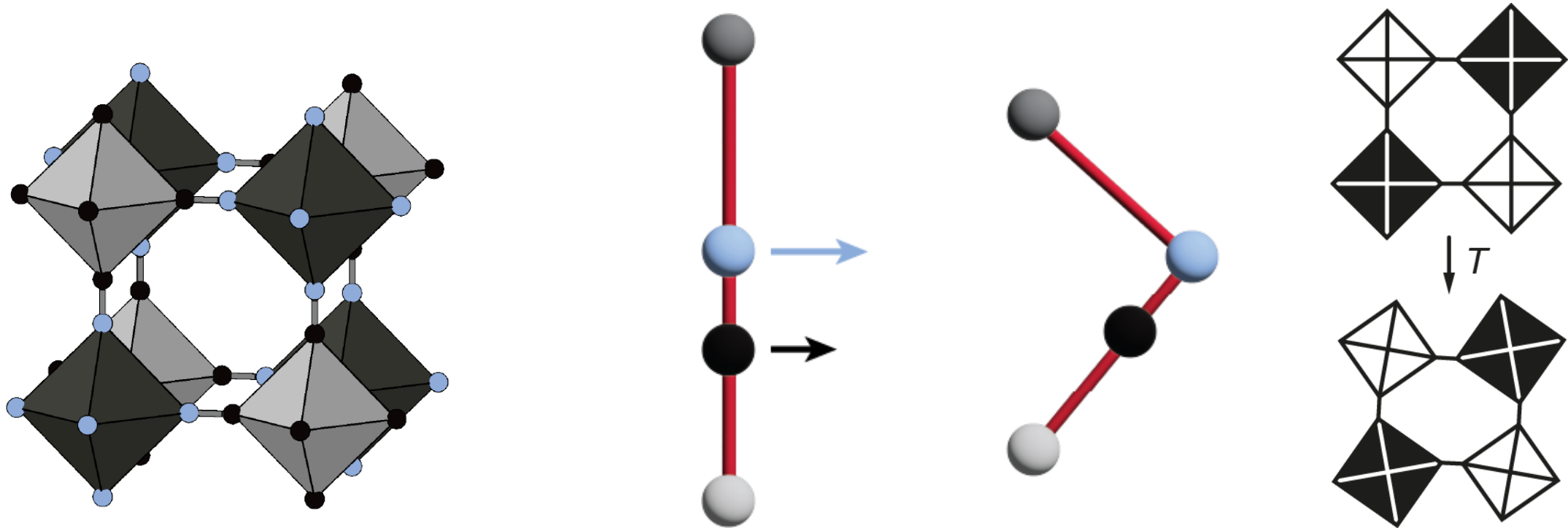
Negative Thermal Expansion (NTE) in $\text{MPt}(\text{CN})_6$ PBAs



A. L. Goodwin, K. W. Chapman, C. J. Kepert, *J. Am. Chem. Soc.*, 2005, 127, 17980

K. W. Chapman, P. J. Chupas, C. J. Kepert, *J. Am. Chem. Soc.*, 2006, 128, 7009—7014

Negative Thermal Expansion (NTE) in $\text{MPt}(\text{CN})_6$ PBAs



A. L. Goodwin, K. W. Chapman, C. J. Kepert, *J. Am. Chem. Soc.*, 2005, 127, 17980

K. W. Chapman, P. J. Chupas, C. J. Kepert, *J. Am. Chem. Soc.*, 2006, 128, 7009—7014

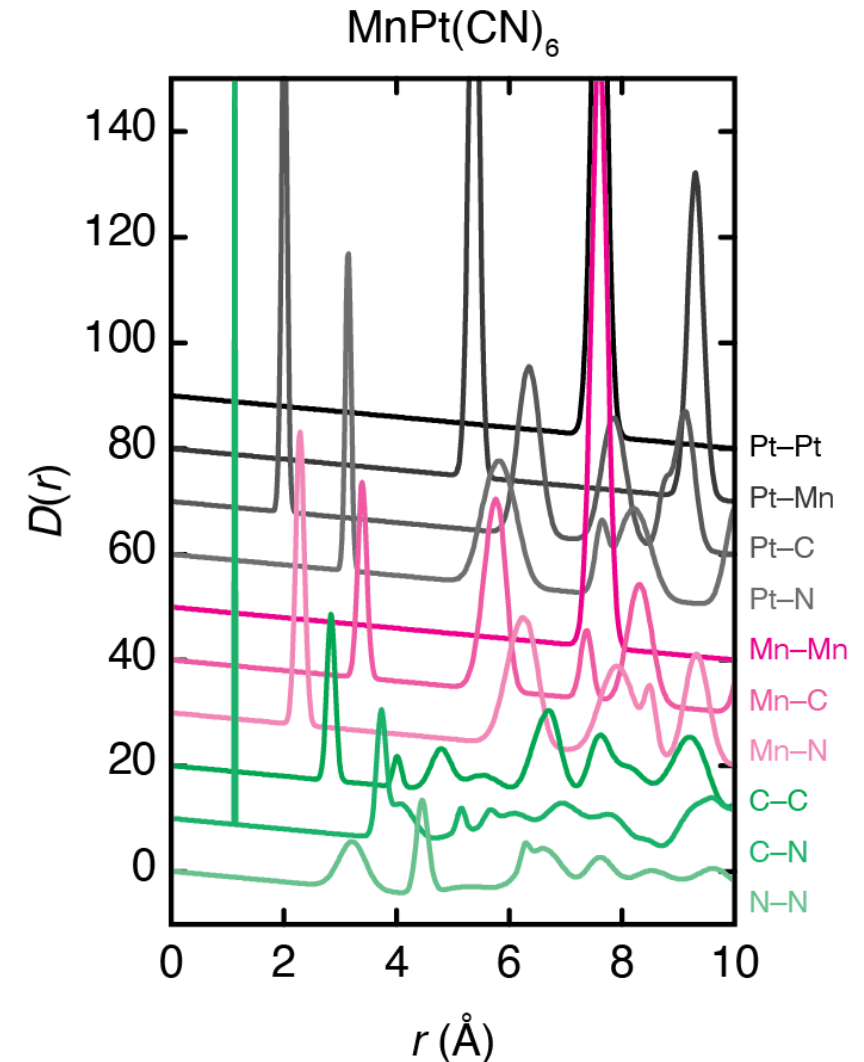
Pair Distribution Function measurements

Understanding local structure

- PDF measurements can provide an excellent experimental handle on **local structure**
- Conventional PDF refinements using monotonic r -dependent peak widths often not suitable for PBAs
- Mixture of **broad and sharp features** for different pair correlations at **similar separations**

K. W. Chapman, P. J. Chupas, C. J. Kepert, *J. Am. Chem. Soc.*, 2005, 127, 11232–11233

N. Ma, R. Ohtani, H. M. Le, S. S. Sørensen, R. Ishikawa, S. Kawata, S. Bureekaew, S. Kosasang, Y. Kawazoe, K. Ohara, M. M. Smedskjaer, S. Horike, *Nat. Commun.*, 2022, 13, 4023



E. A. Harbourne, H. Barker, Q. Guérault, J. Cattermull, L. A. V. Nagle-Cocco, N. Roth, J. S. O. Evans, D. A. Keen, A. L. Goodwin, *Chem. Mater.*, 2024, 36, 5796

Constrained big-box modelling

We have developed a modified “interaction-space” PDF refinement approach.

Based on the iterative refinement of parameters of an empirical lattice dynamical model against the experimental PDF data.

RMC

Move/swap
atoms



Fit data

Constrained “RMC” cf EPSR

Change interatomic
potentials



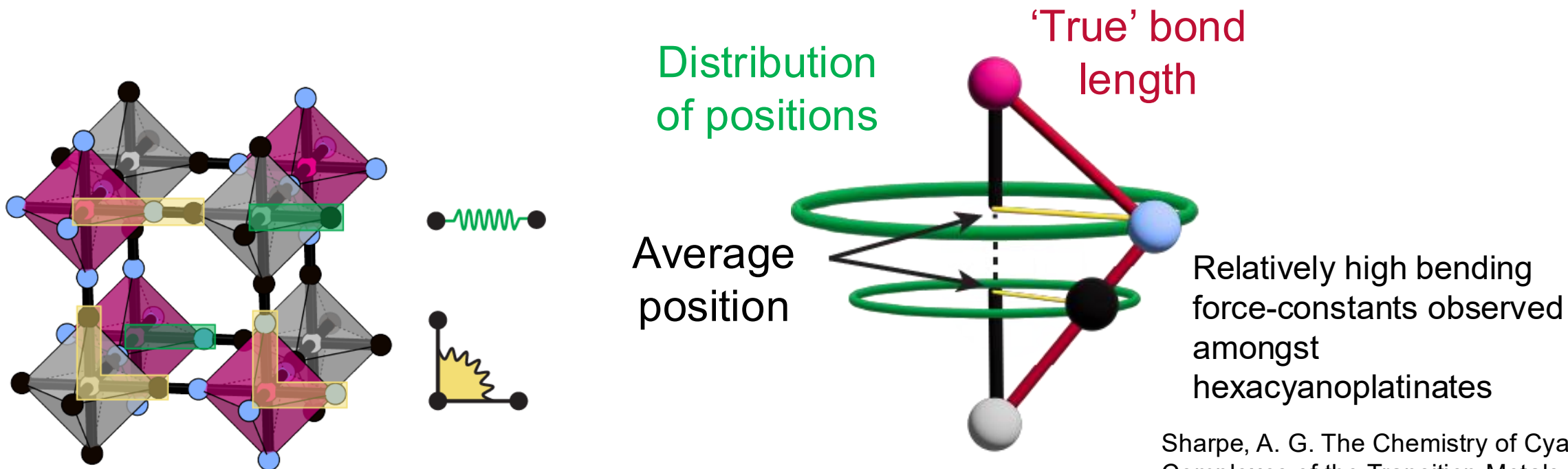
Calculate atom
positions with MC



Fit data (with TOPAS)

MC-driven empirical potential approach

$$E = \frac{1}{2} \sum_{\text{bonds}} k_r (r - r_e)^2 + \frac{1}{2} \sum_{\text{angles}} k_\theta (\theta - \theta_e)^2$$

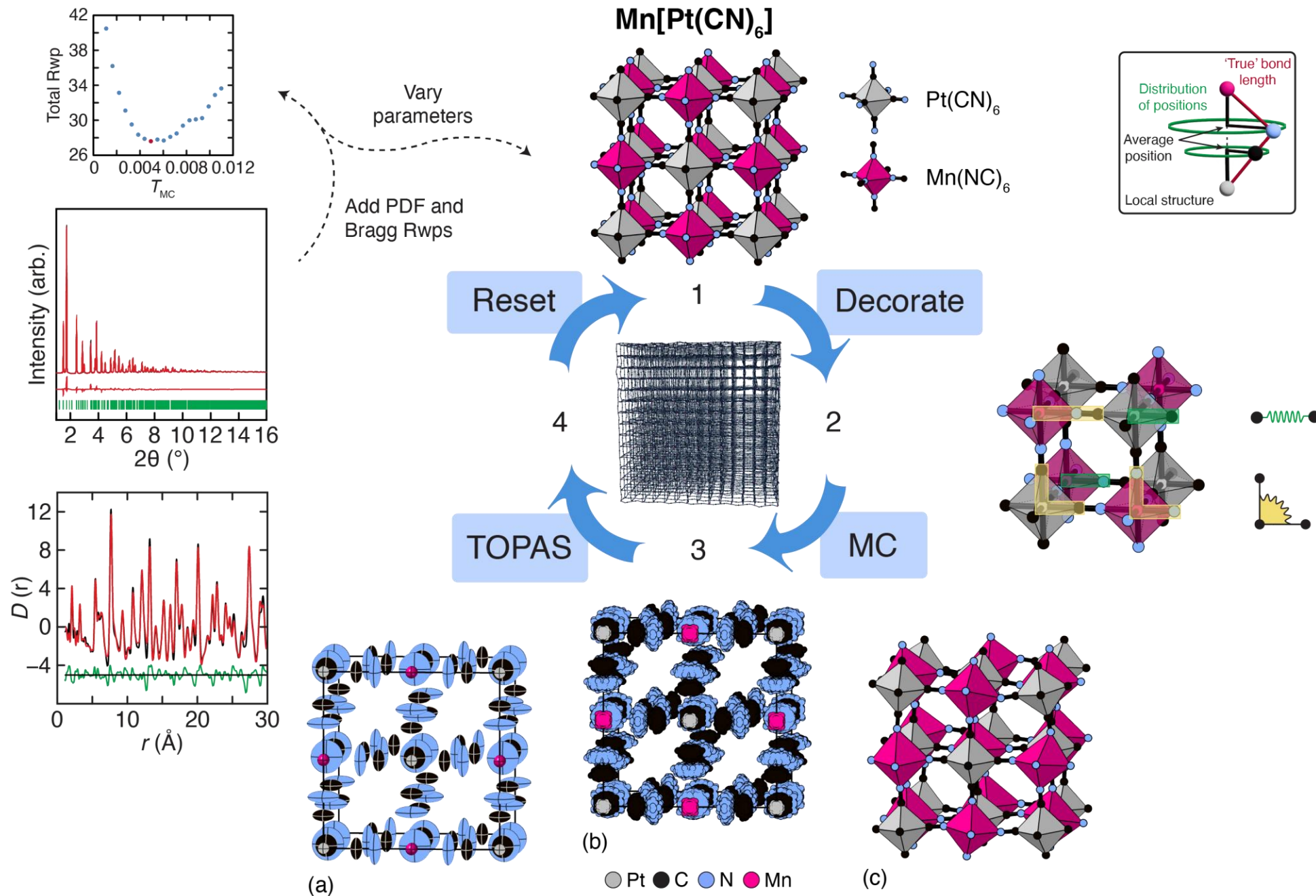


Sharpe, A. G. *The Chemistry of Cyano Complexes of the Transition Metals*; Academic Press: London, 1976.

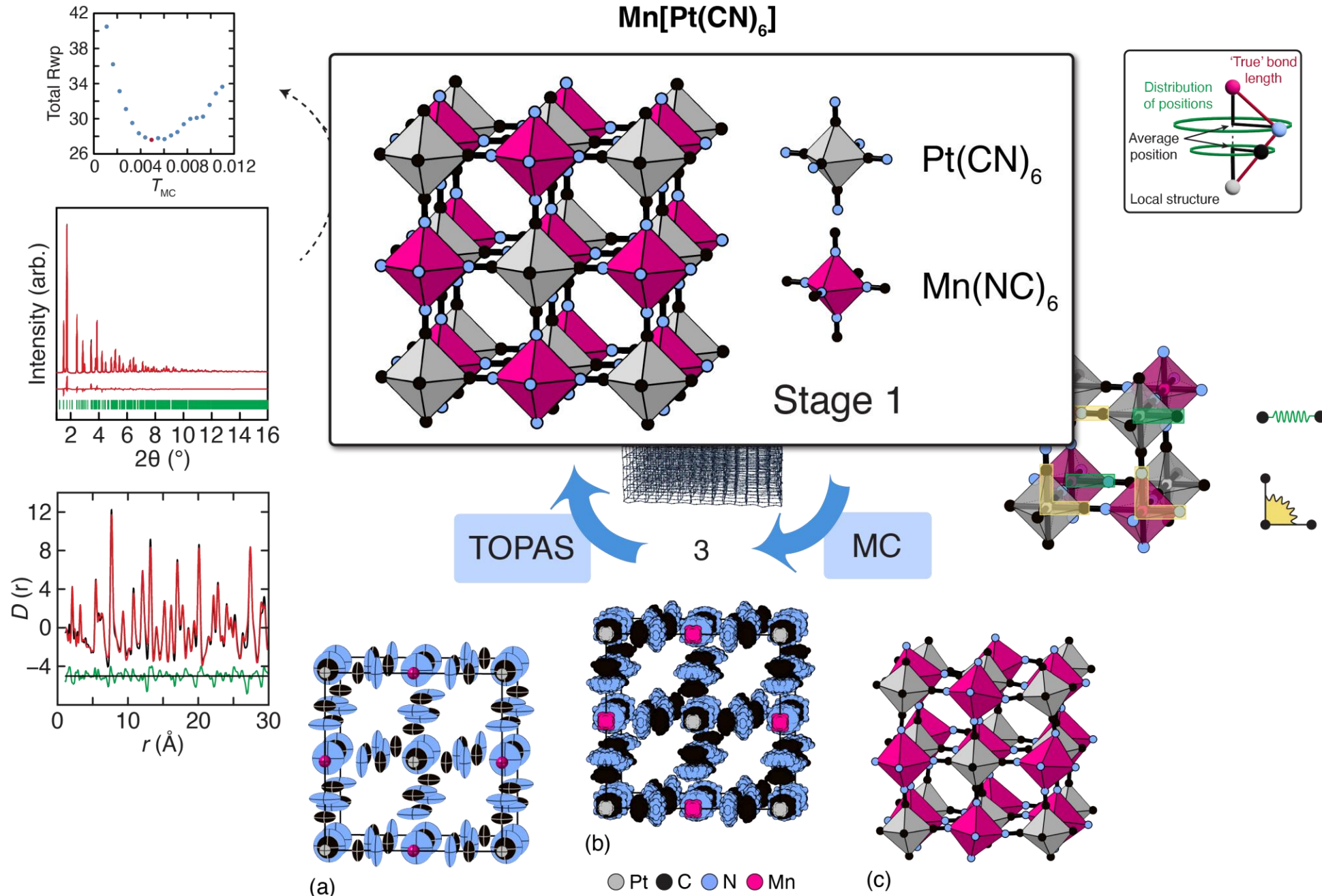
A. L. Goodwin, K. W. Chapman, C. J. Kepert, *J. Am. Chem. Soc.*, 2005, 127, 17980

K. W. Chapman, P. J. Chupas, C. J. Kepert, *J. Am. Chem. Soc.*, 2006, 128, 7009—7014

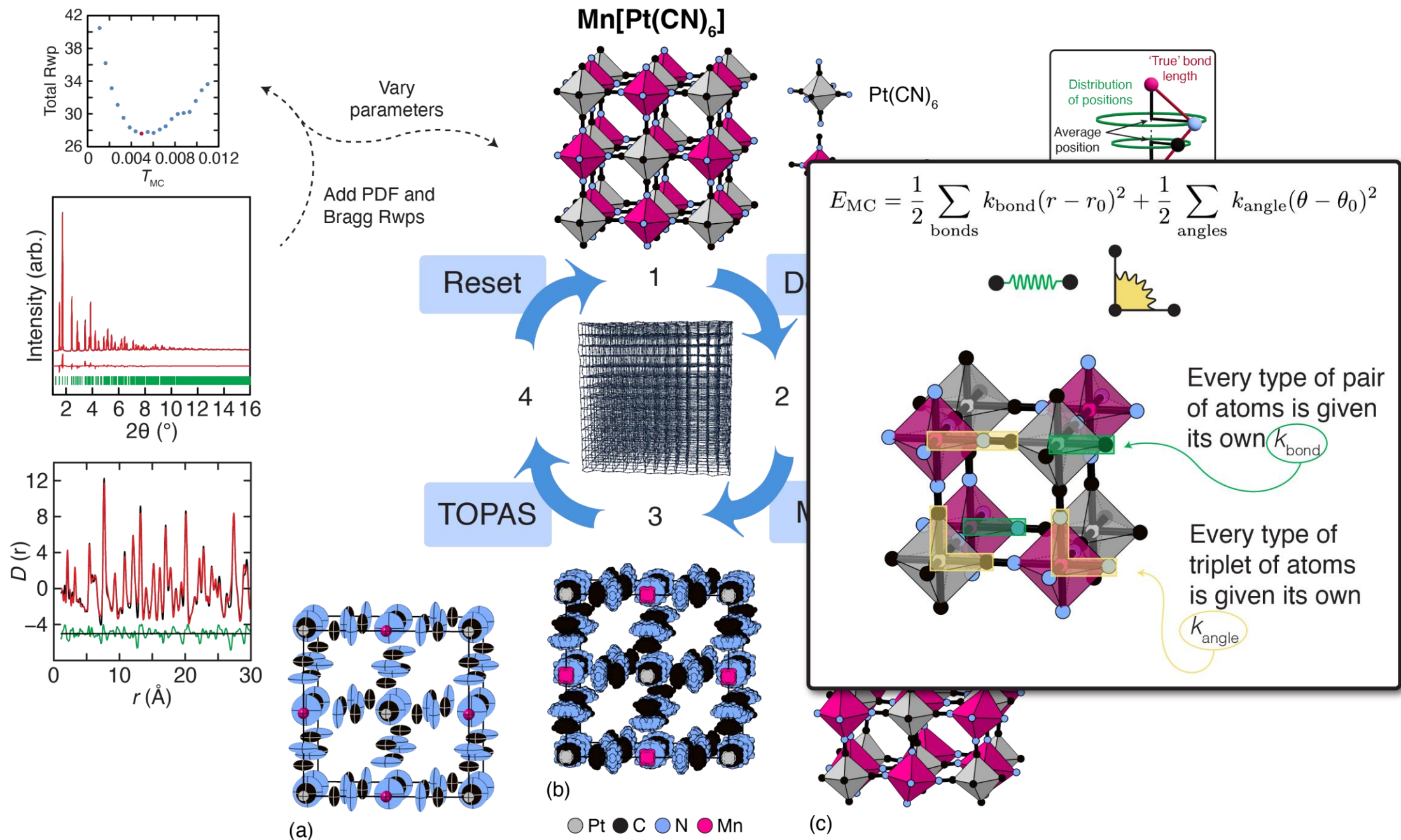
'Interaction-space' MC-driven big-box modelling approach



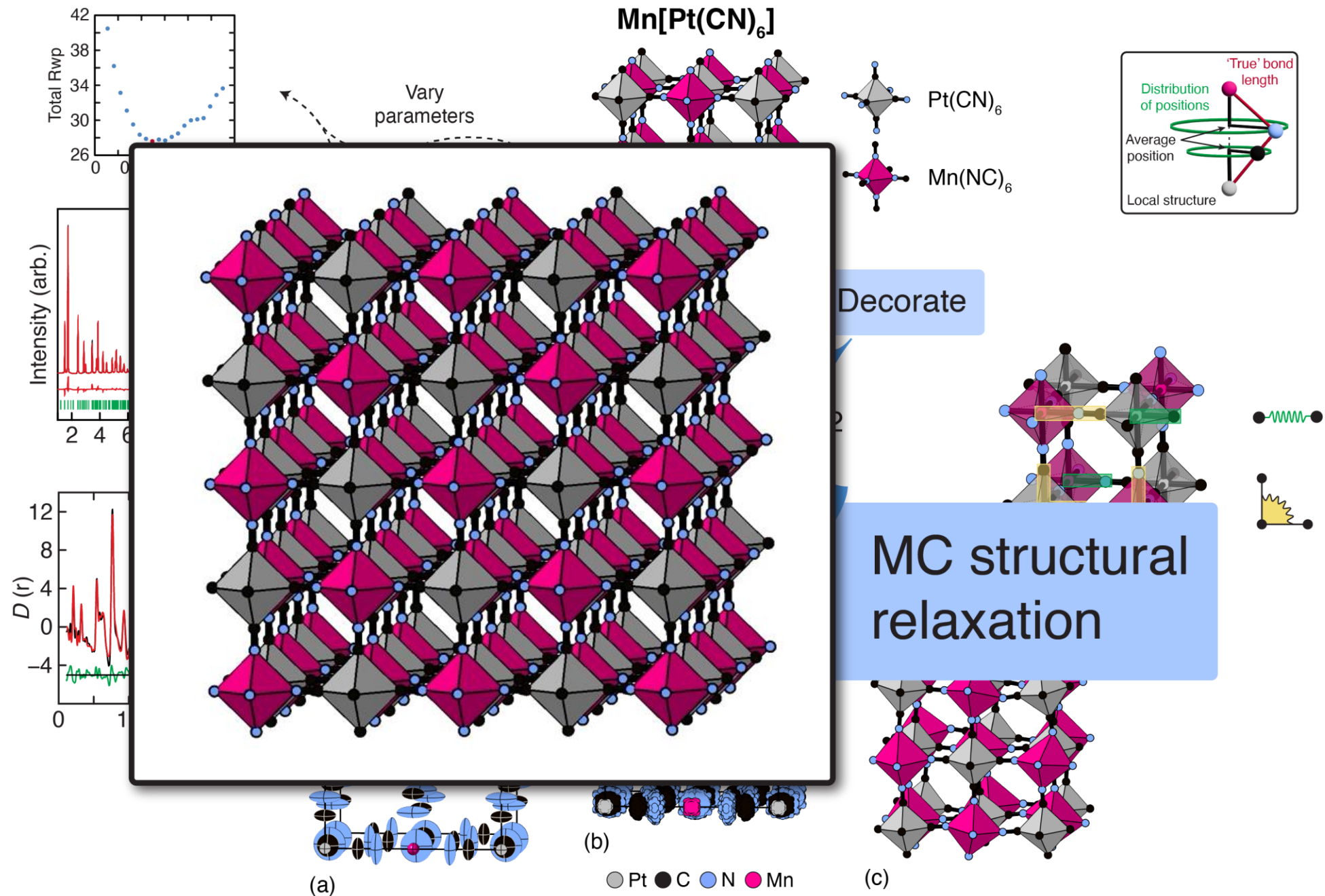
'Interaction-space' MC-driven big-box modelling approach



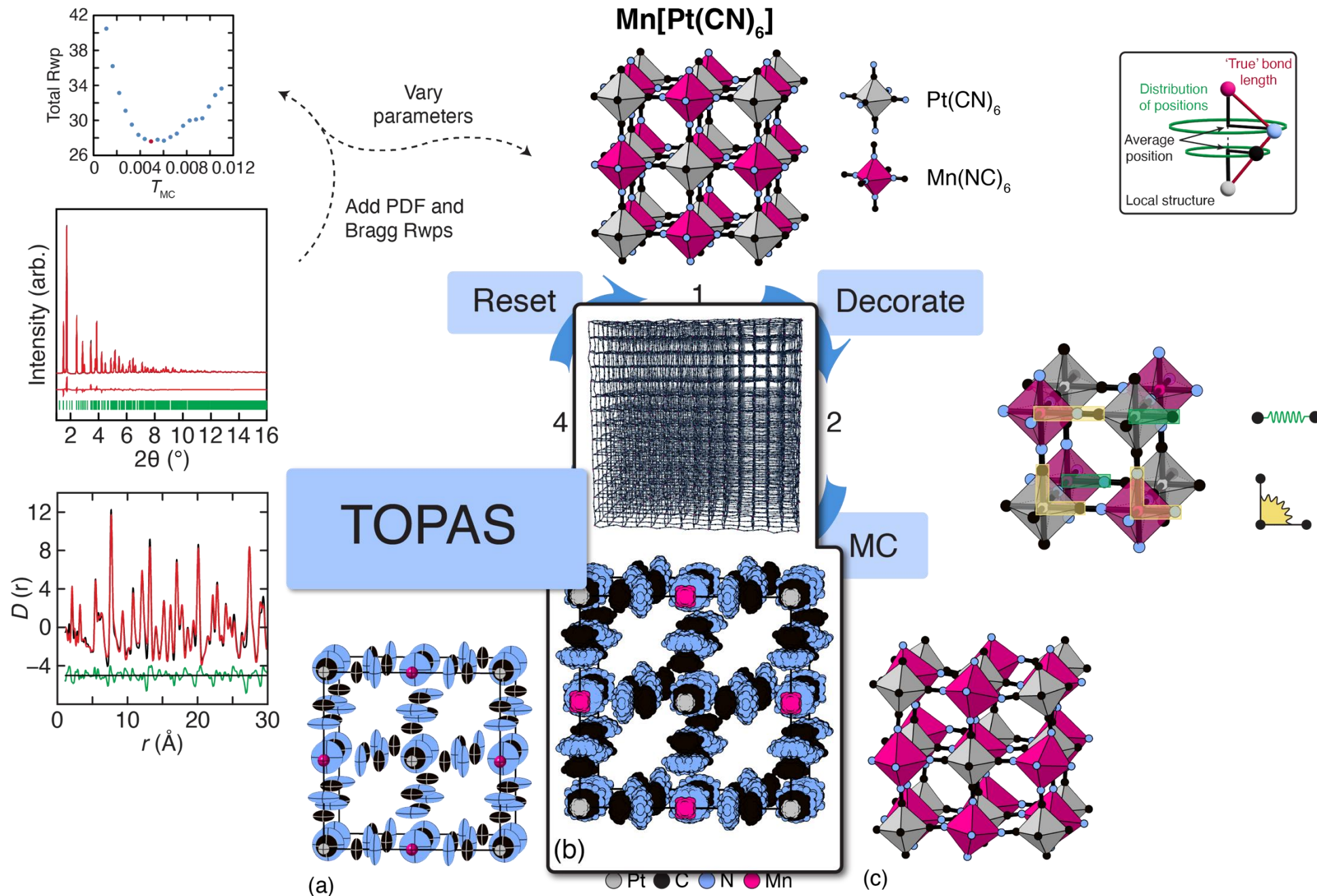
'Interaction-space' MC-driven big-box modelling approach



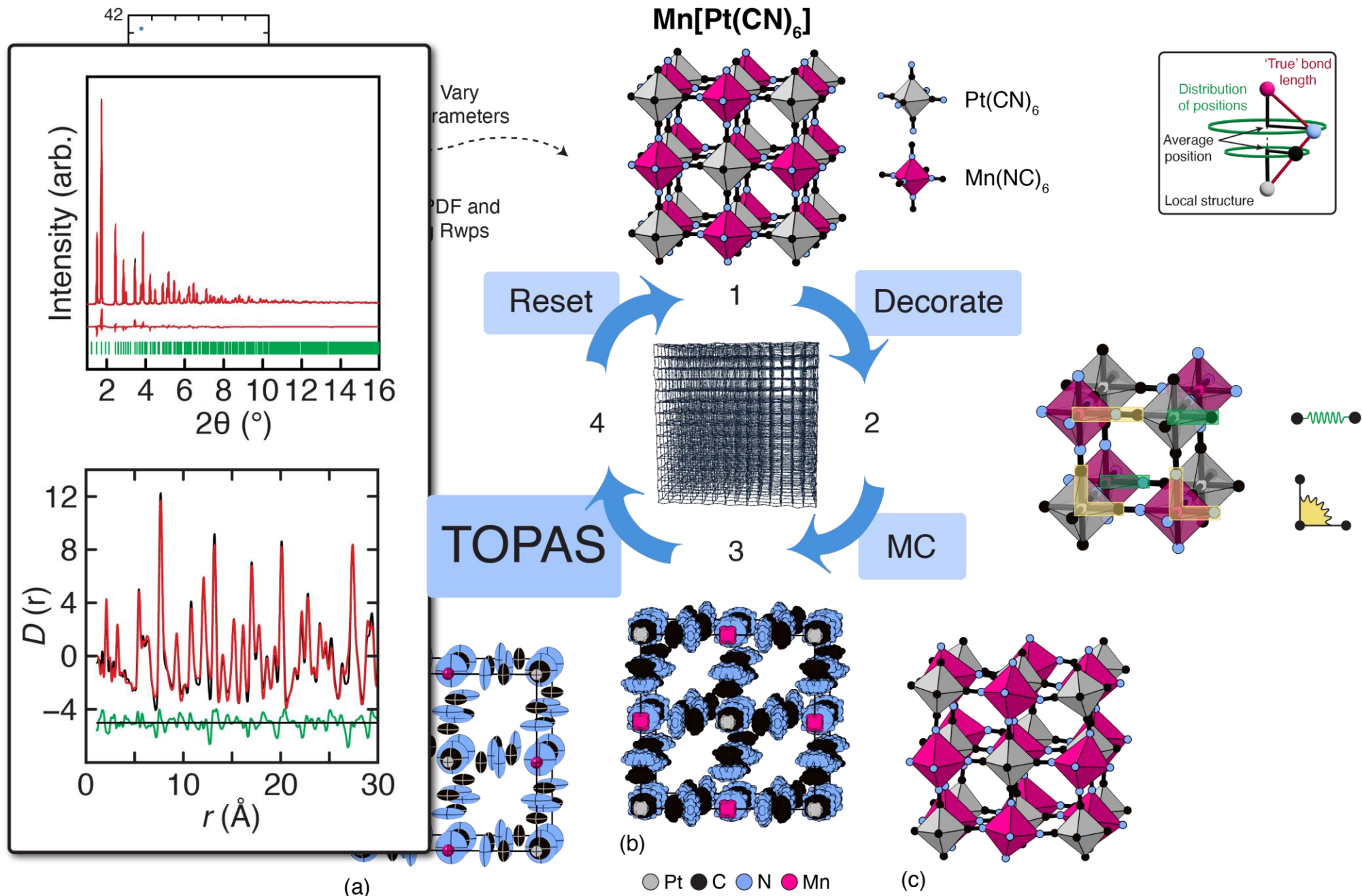
'Interaction-space' MC-driven big-box modelling approach



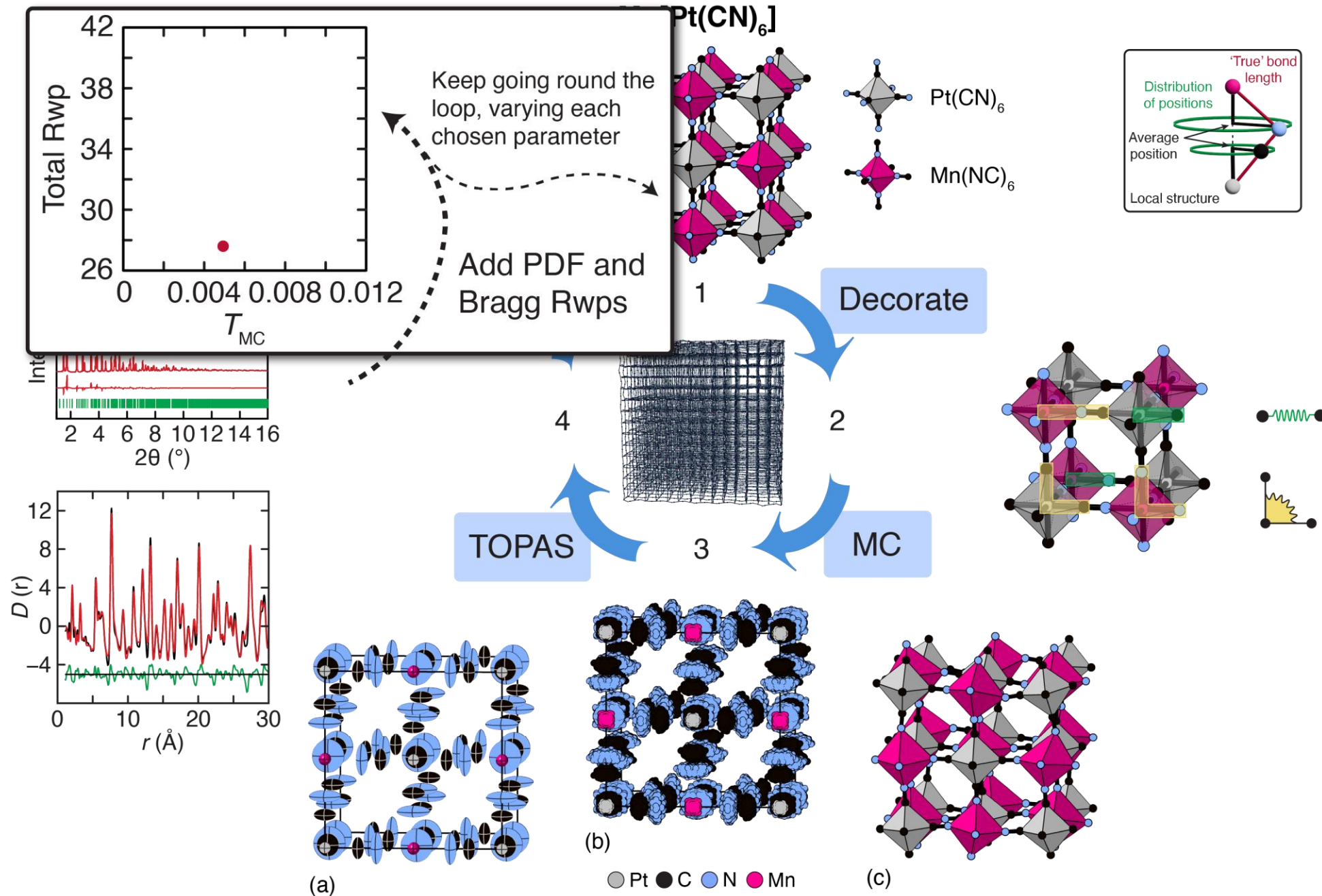
'Interaction-space' MC-driven big-box modelling approach



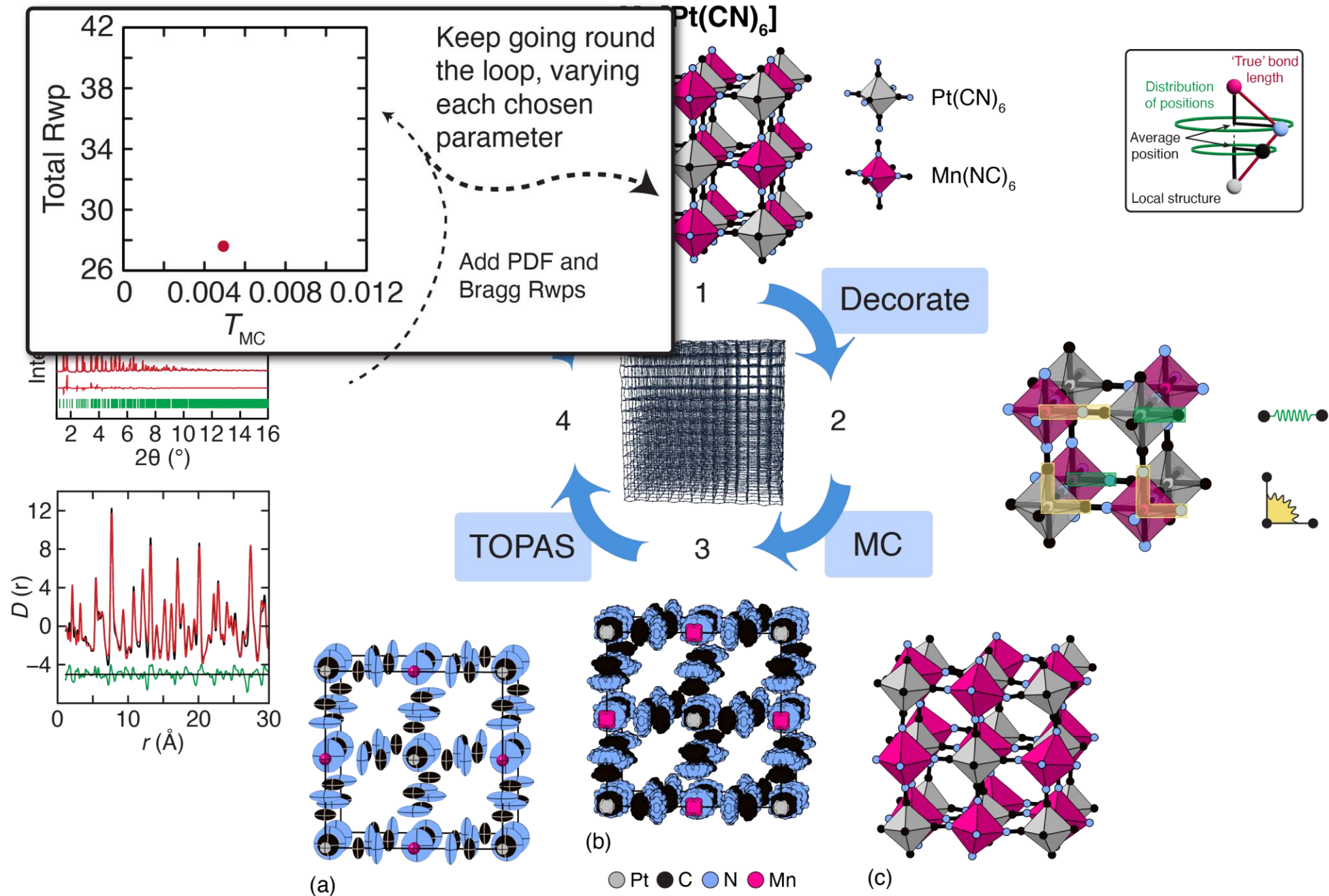
'Interaction-space' MC-driven big-box modelling approach



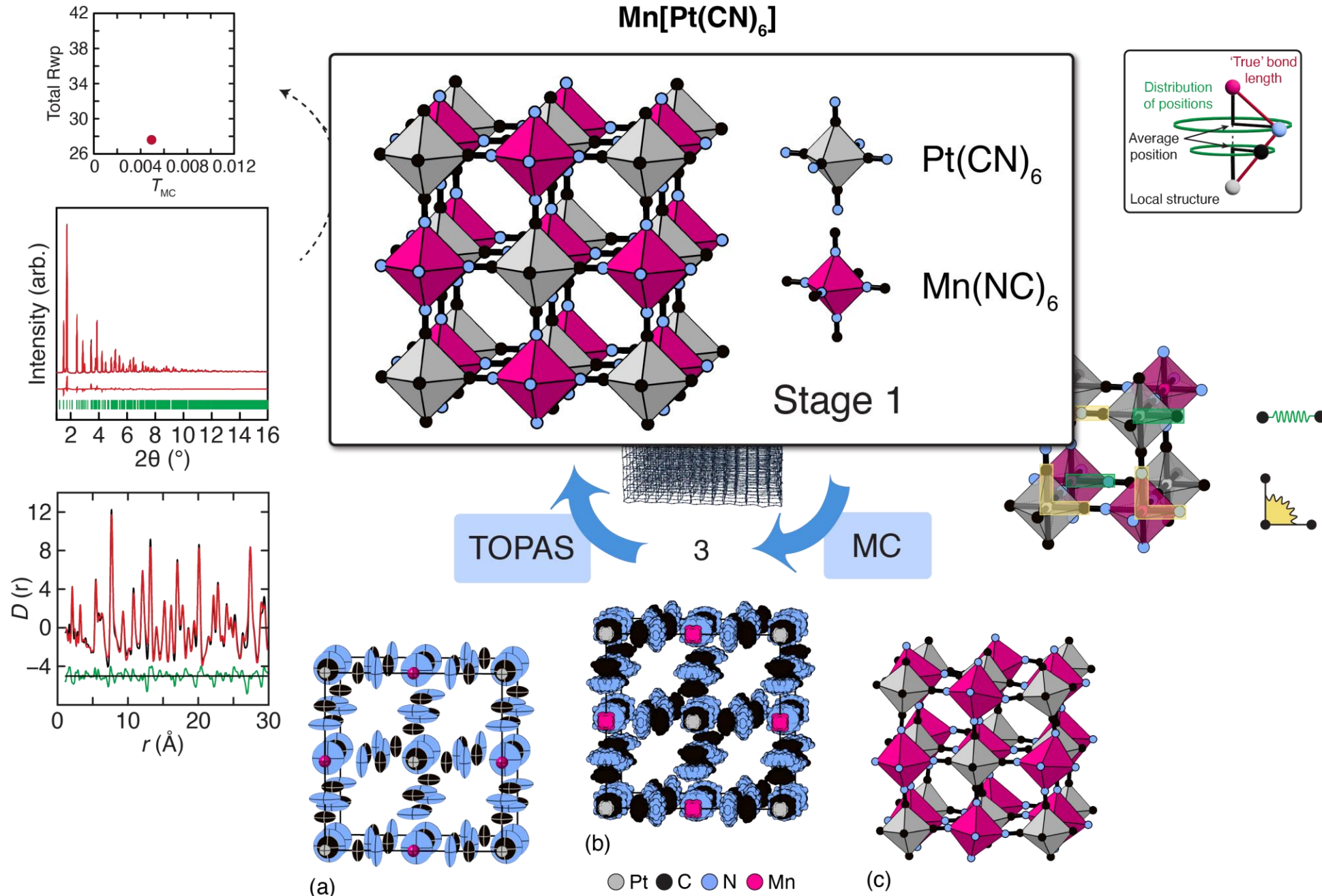
'Interaction-space' MC-driven big-box modelling approach



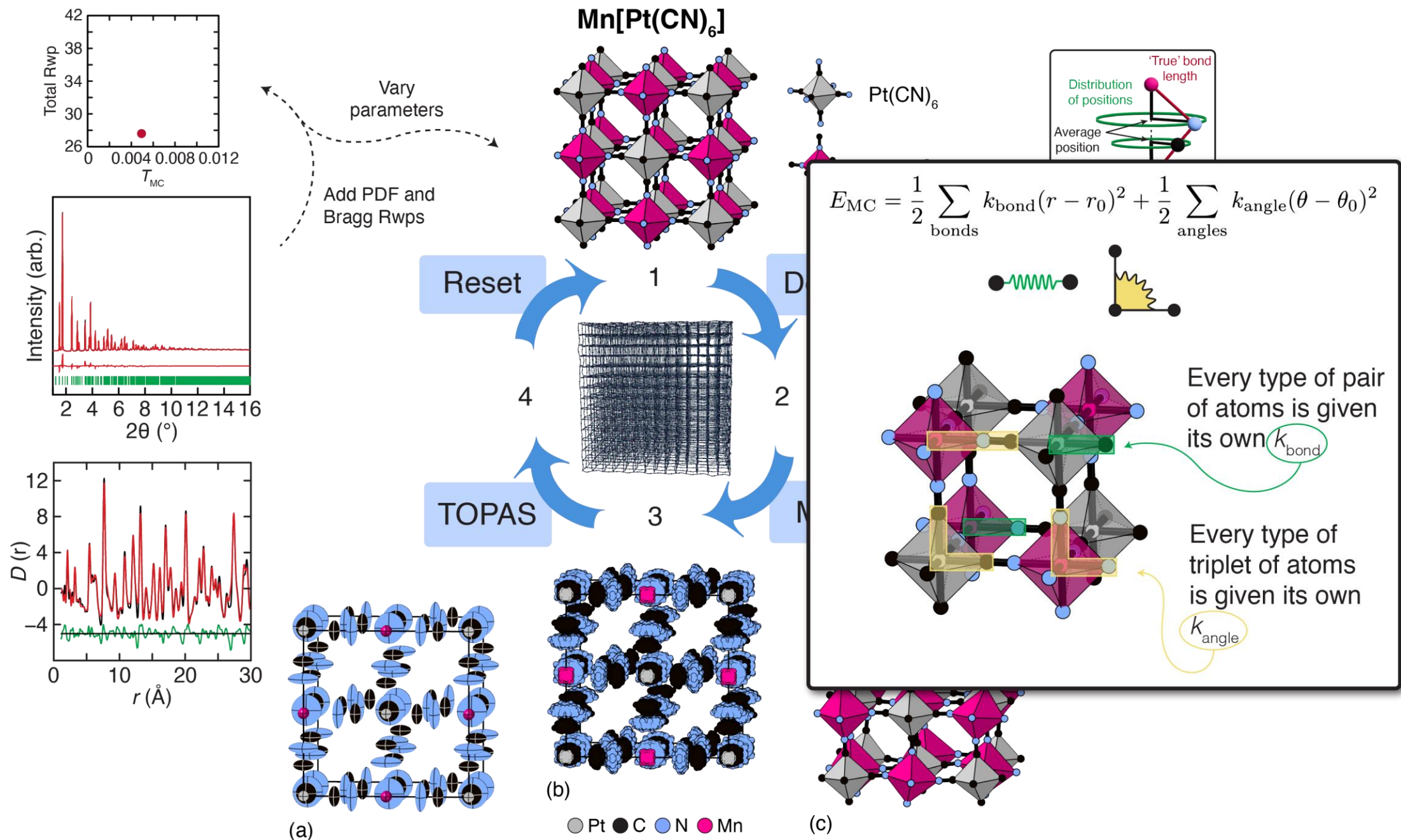
'Interaction-space' MC-driven big-box modelling approach



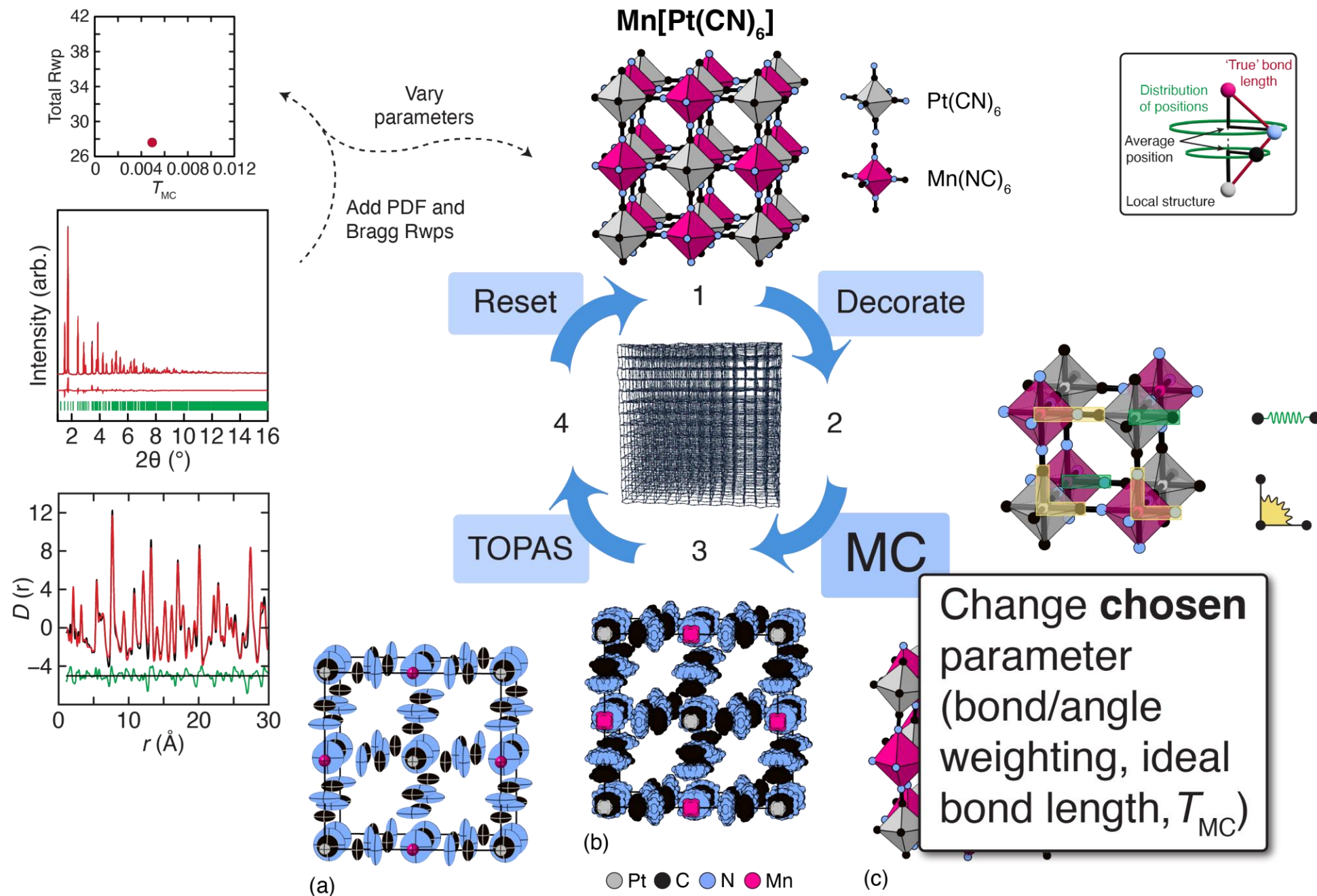
'Interaction-space' MC-driven big-box modelling approach



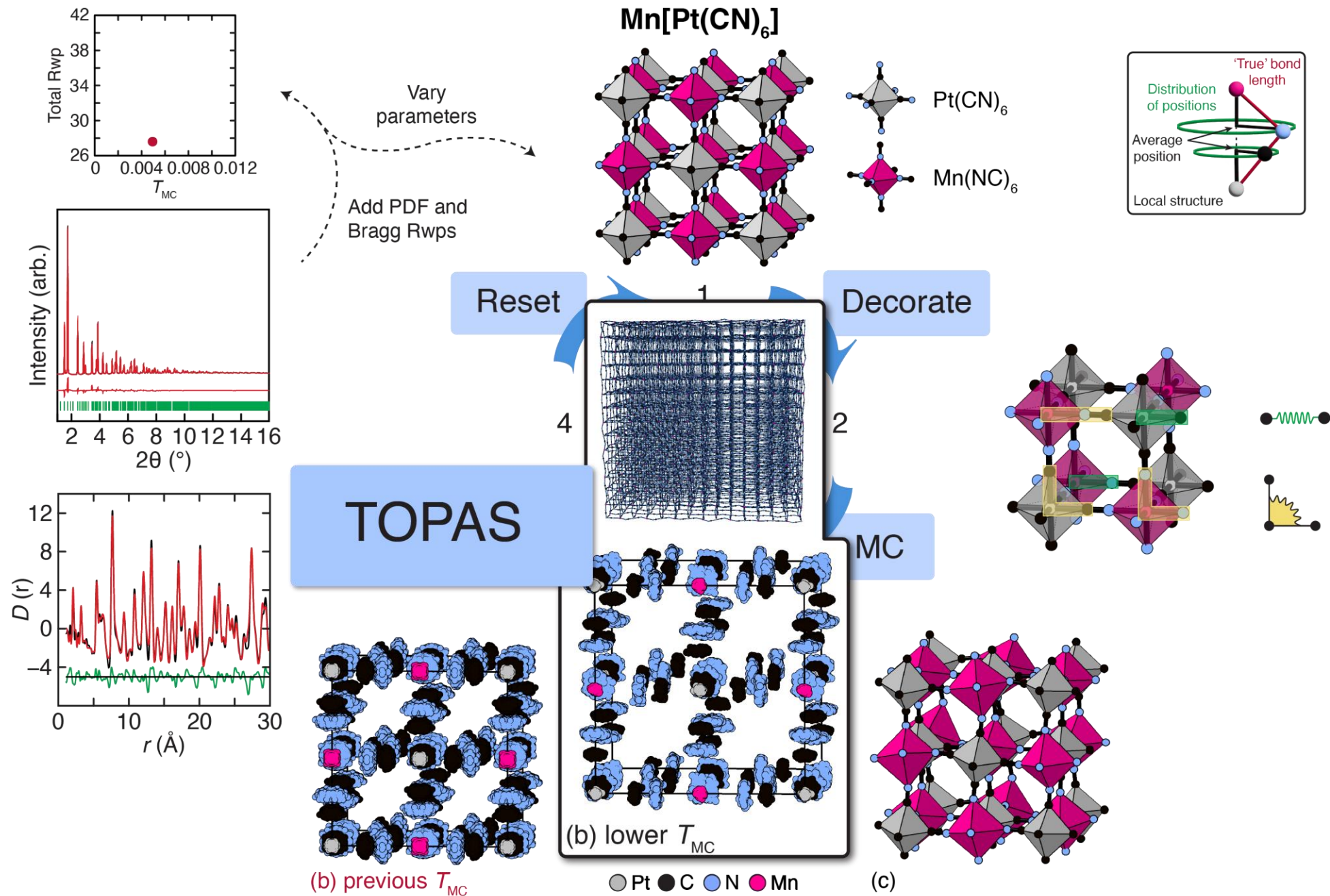
'Interaction-space' MC-driven big-box modelling approach



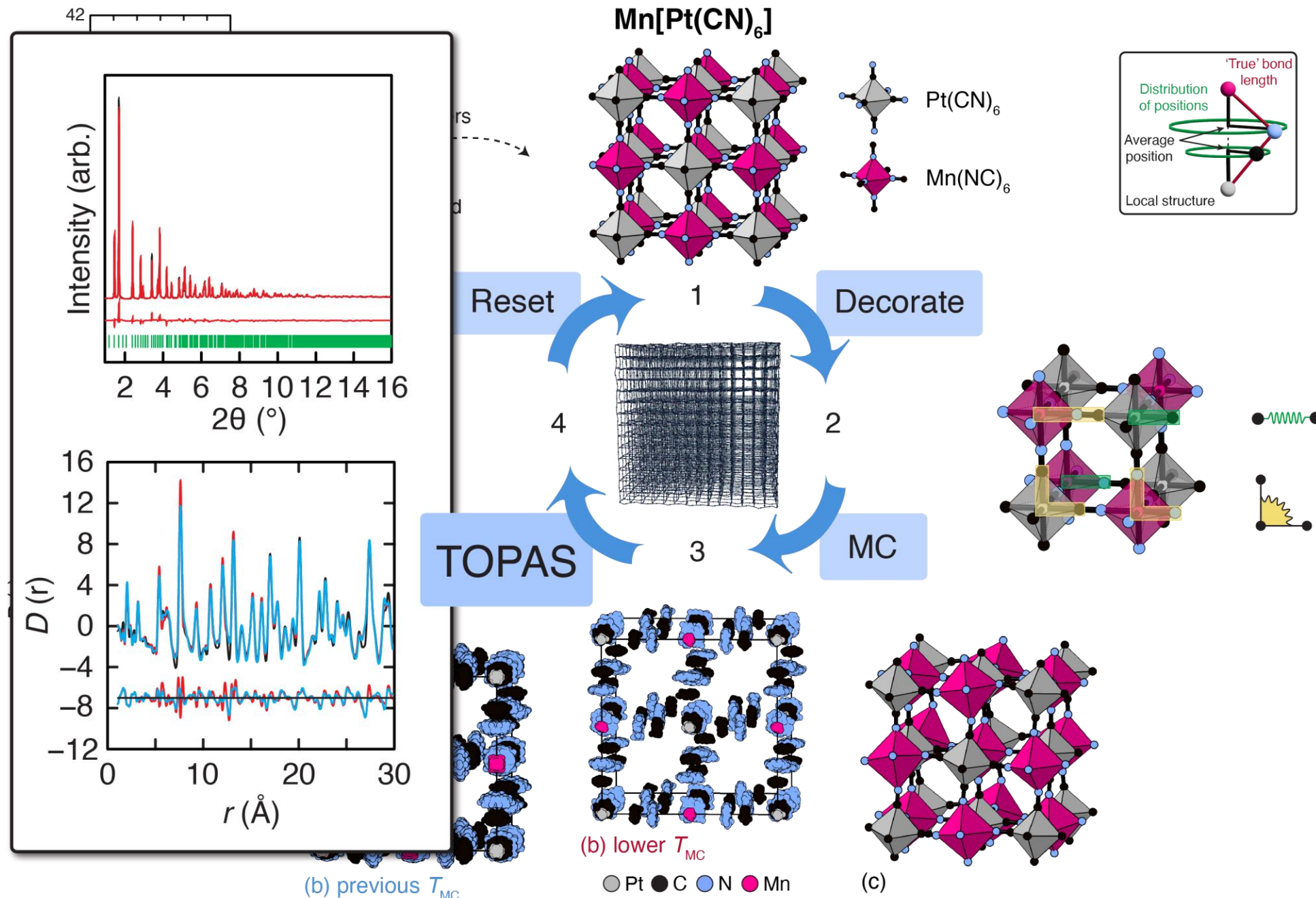
'Interaction-space' MC-driven big-box modelling approach



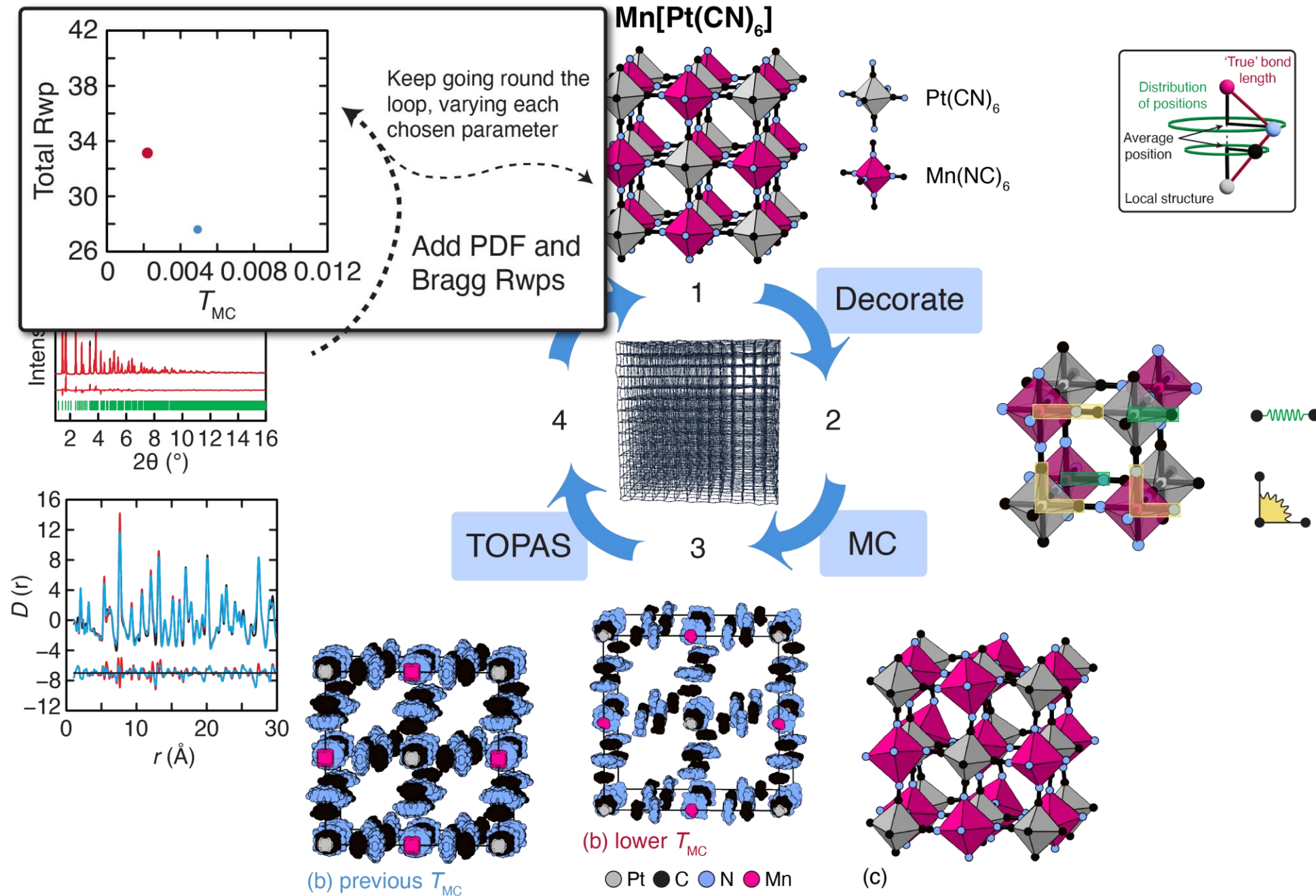
'Interaction-space' MC-driven big-box modelling approach



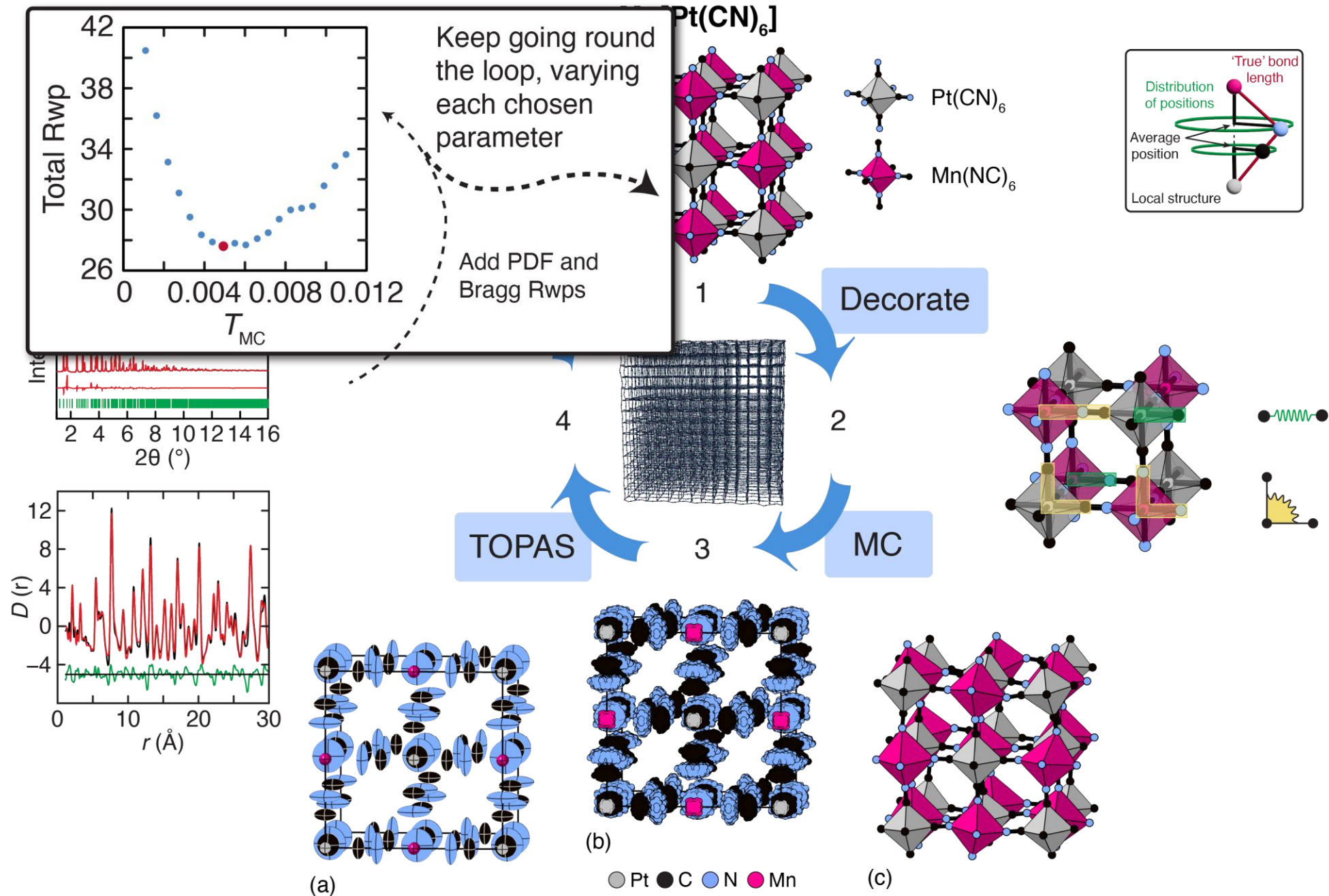
'Interaction-space' MC-driven big-box modelling approach



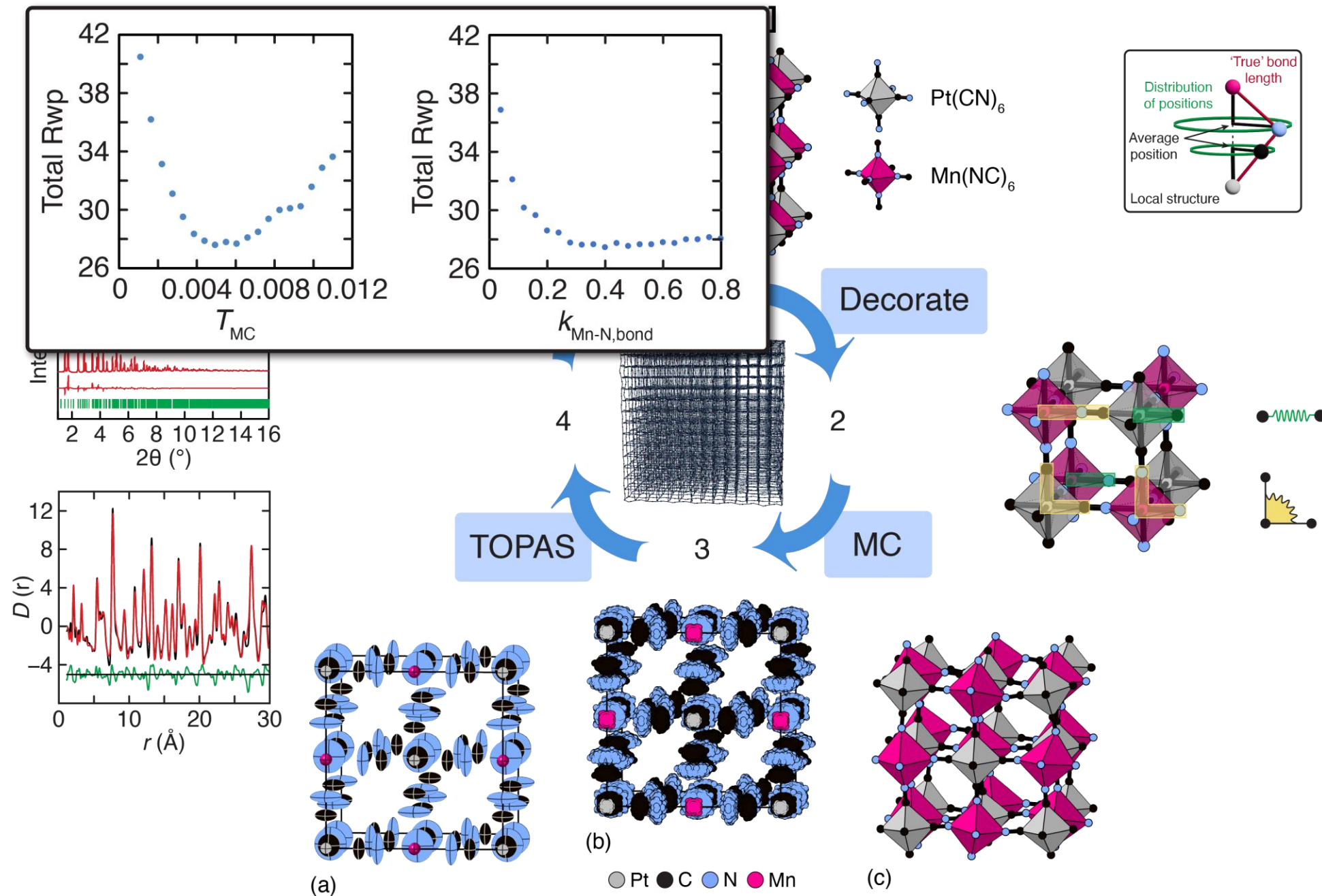
'Interaction-space' MC-driven big-box modelling approach



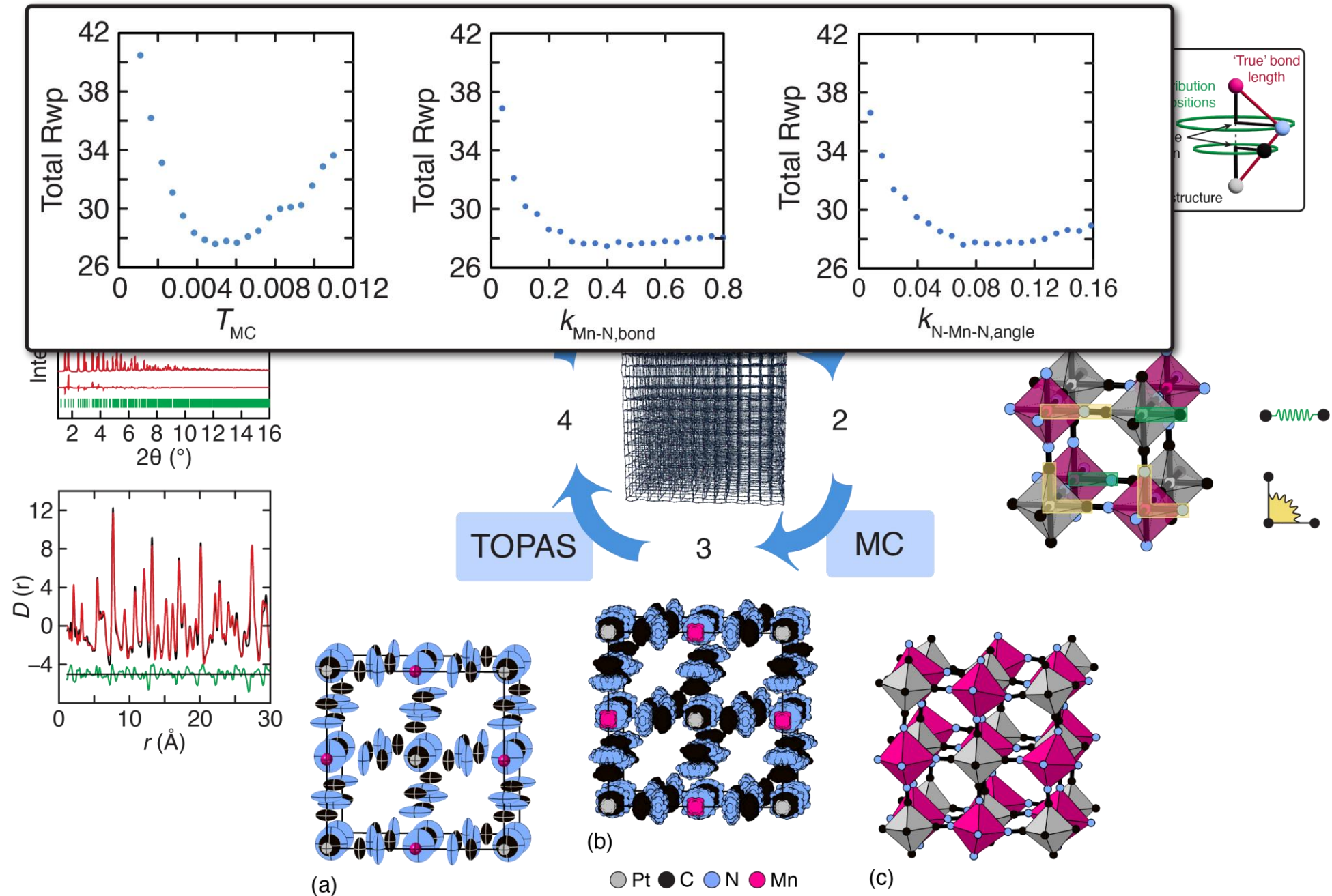
'Interaction-space' MC-driven big-box modelling approach



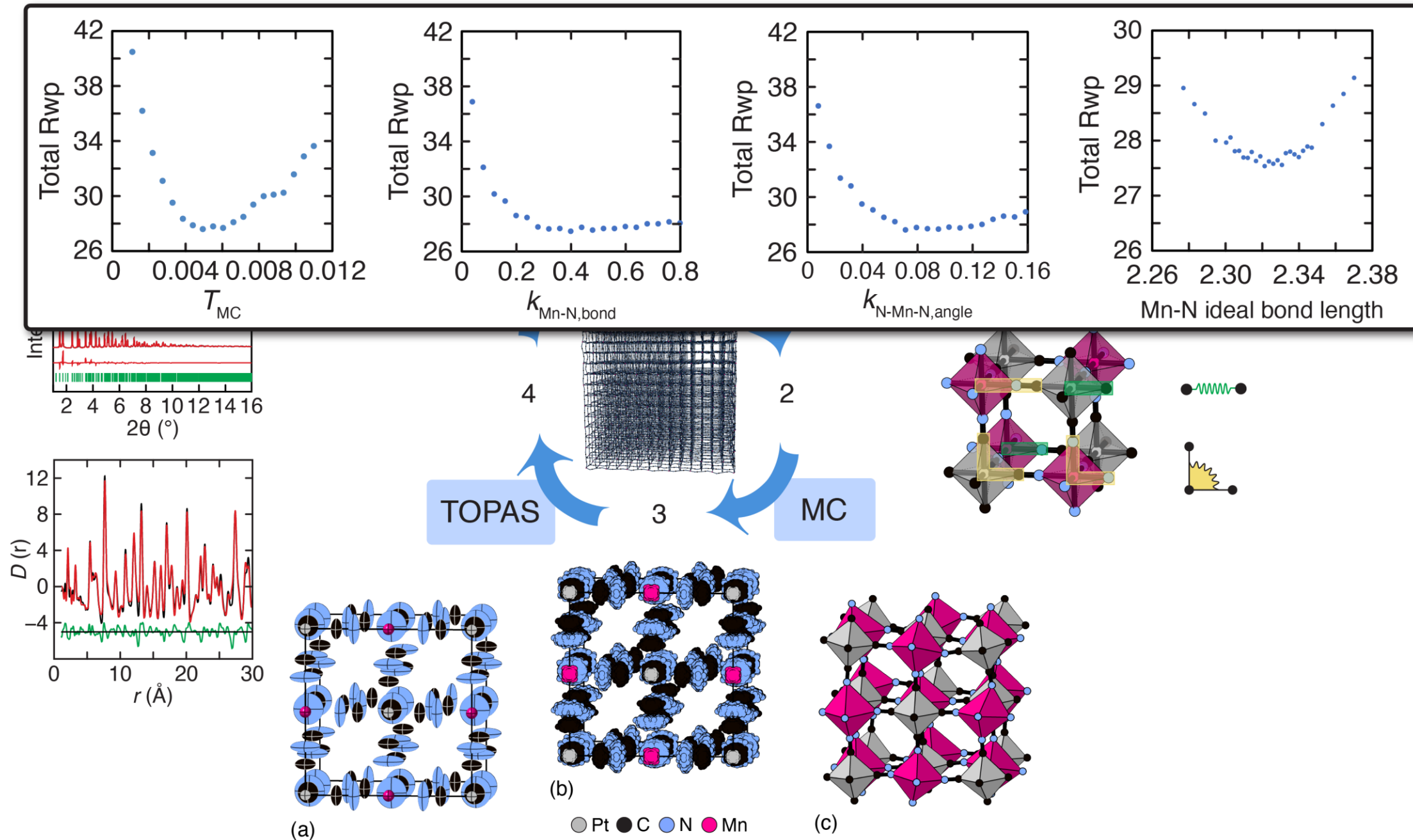
'Interaction-space' MC-driven big-box modelling approach



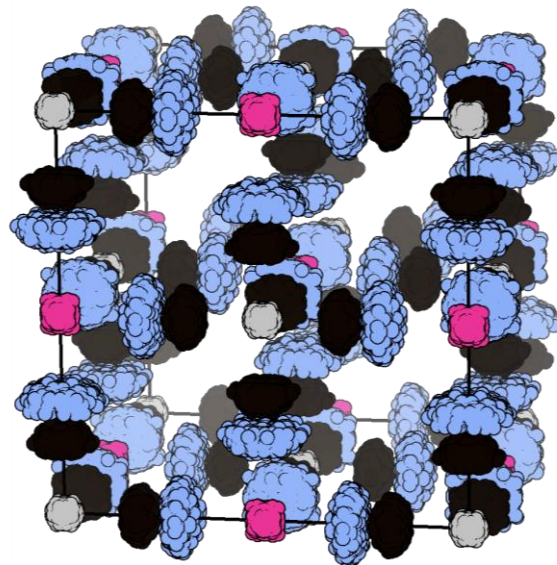
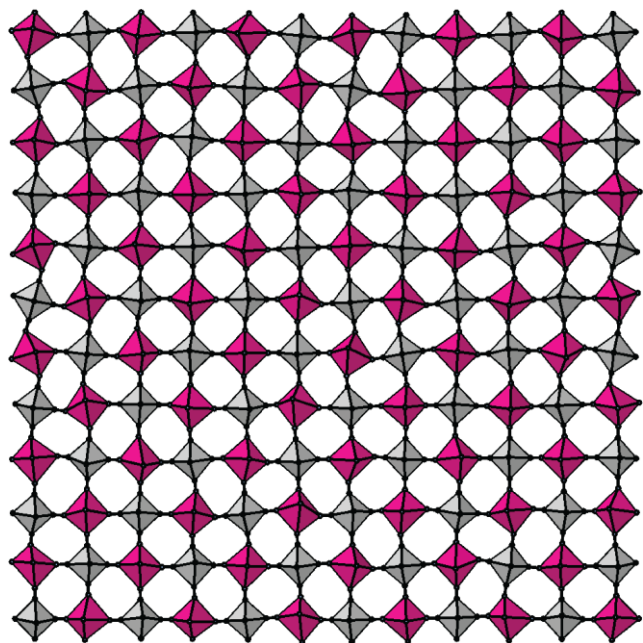
'Interaction-space' MC-driven big-box modelling approach



'Interaction-space' MC-driven big-box modelling approach



'Interaction-space' MC-driven big-box modelling – $\text{MnPt}(\text{CN})_6$



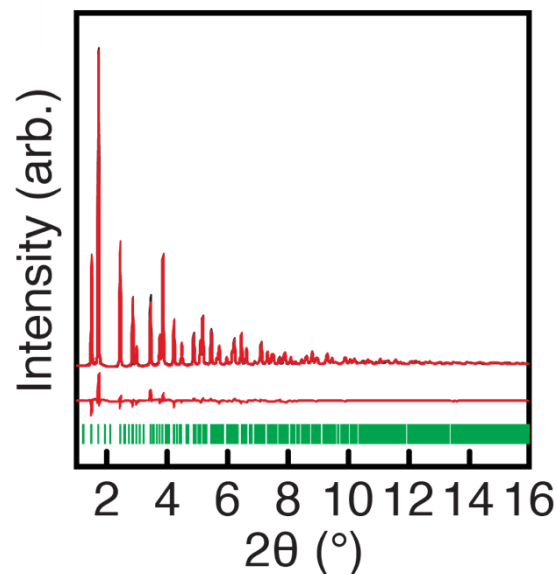
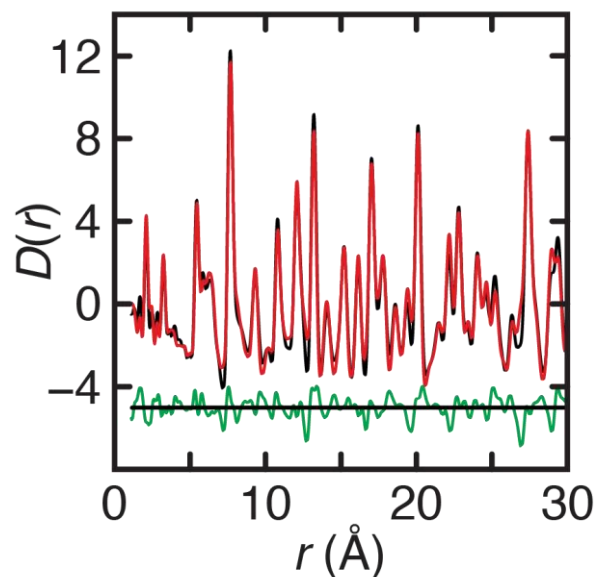
Clear why conventional PDF refinements using monotonic r -dependent peak widths fail:

- The distributions around Mn and Pt are very tightly bunched.

→ The corresponding PDF peaks will be narrow.

- The C/N distributions are very diffuse.

→ Any C/N – C/N peaks will be broader.

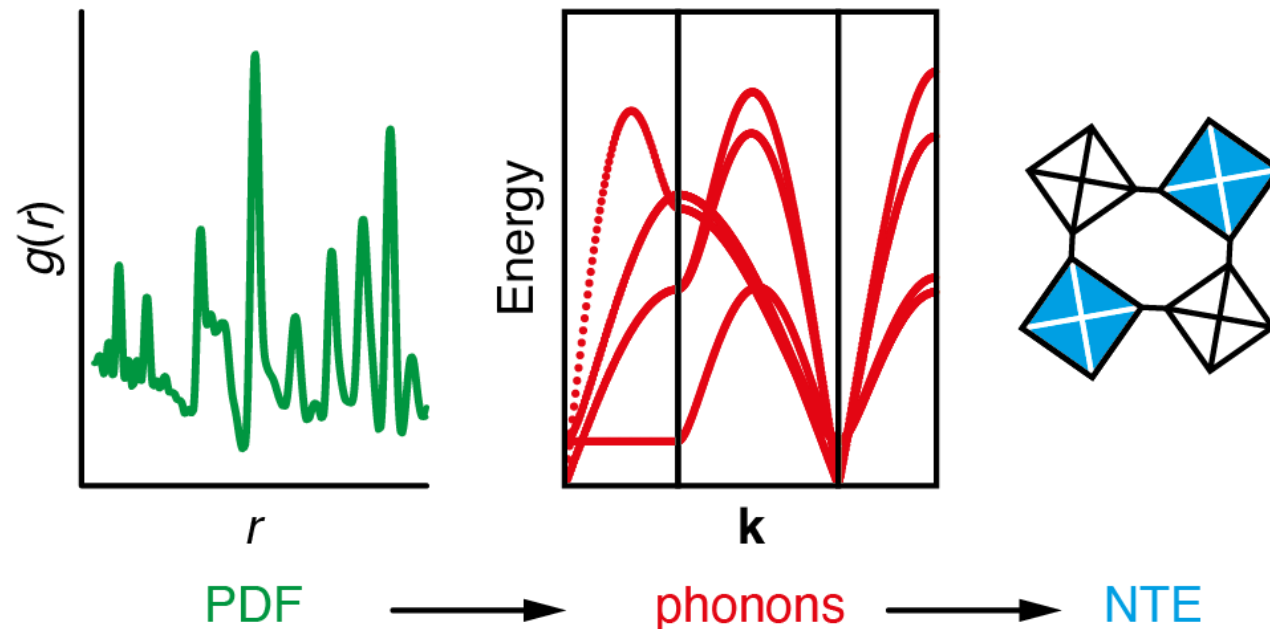


'Interaction-space' MC-driven big-box modelling

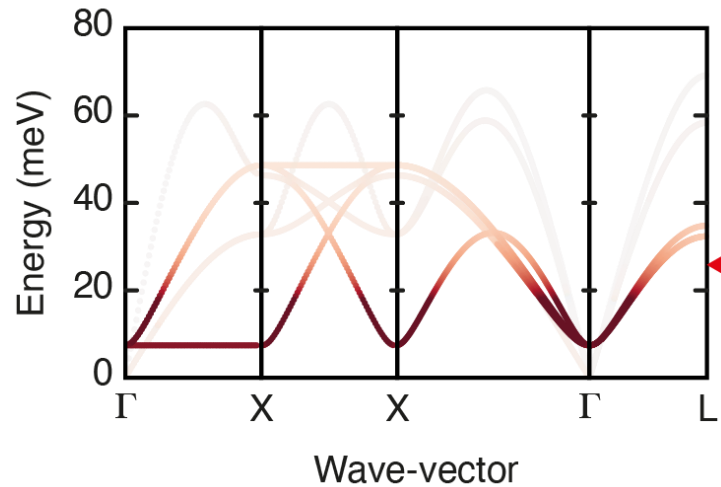
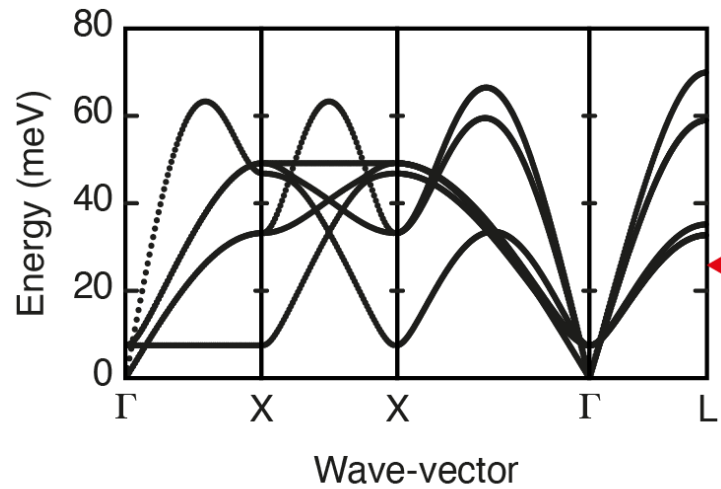
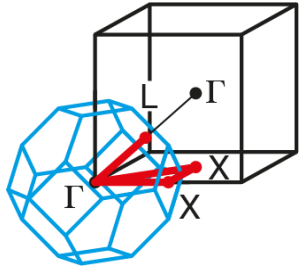
A particular **advantage** of determining **effective potentials** that govern their lattice dynamics – we are able to **identify directly** the likely **phonon modes** most important in **driving NTE**.

Obtain this insight even by fitting data collected at a **single (ambient) temperature**.

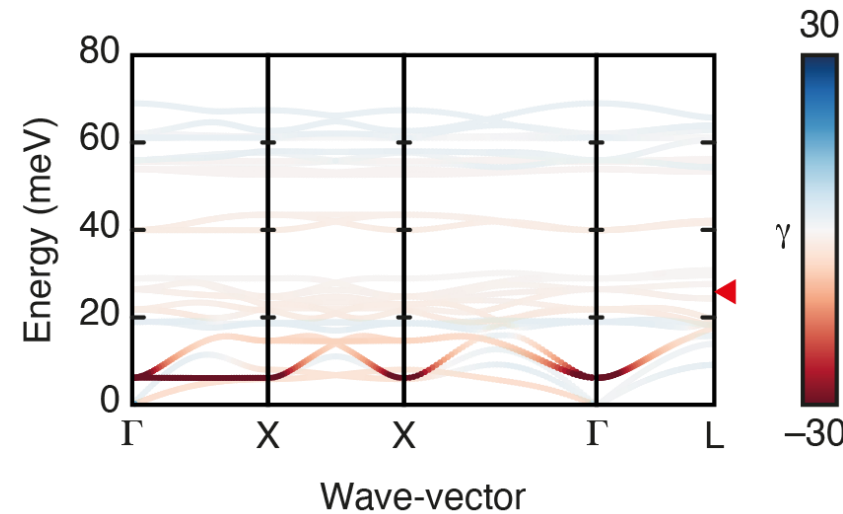
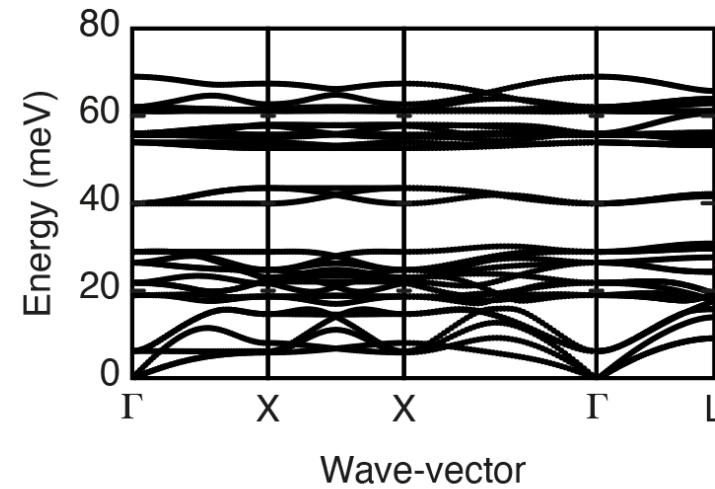
$$E = \frac{1}{2} \sum_{\text{bonds}} k_r (r - r_e)^2 + \frac{1}{2} \sum_{\text{angles}} k_\theta (\theta - \theta_e)^2$$



Lattice dynamical calculations – comparison to DFT $\text{ZnPt}(\text{CN})_6$



Empirical calculations
 $\text{MnPt}(\text{CN})_6$



DFT calculations
 $\text{ZnPt}(\text{CN})_6$

$$\gamma(\mathbf{k}, \nu) = -\frac{\partial \ln \omega(\mathbf{k}, \nu)}{\partial \ln V}$$

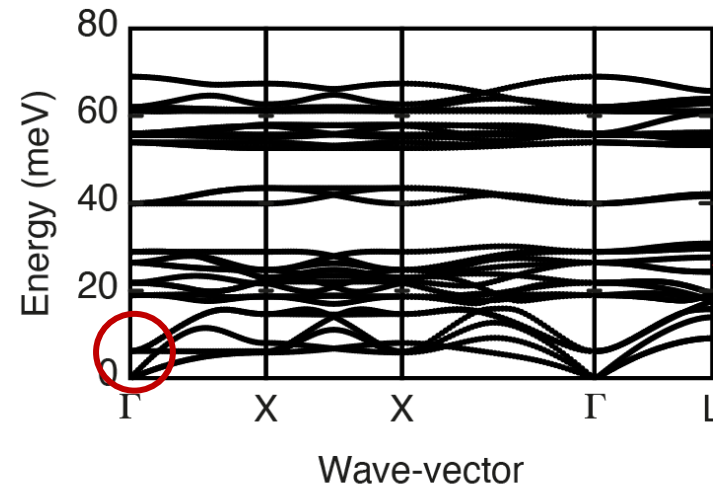
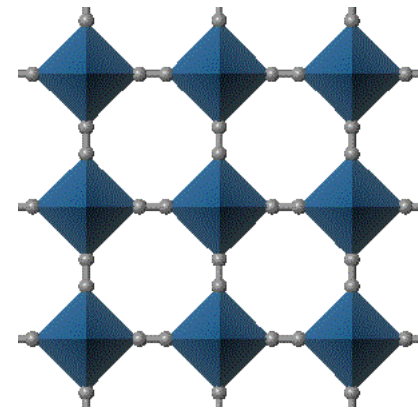
Lattice dynamical calculations – comparison to DFT $\text{ZnPt}(\text{CN})_6$



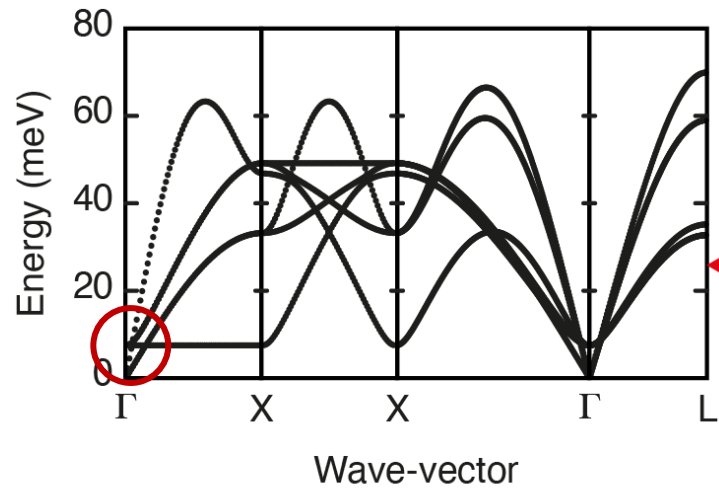
Dispersionless branch

$\mathbf{k} = [00\xi]$ direction from Γ to X

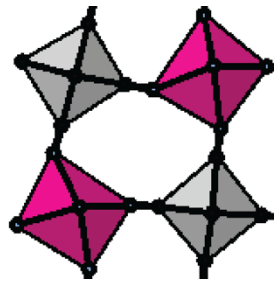
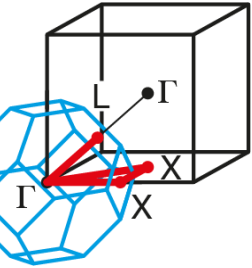
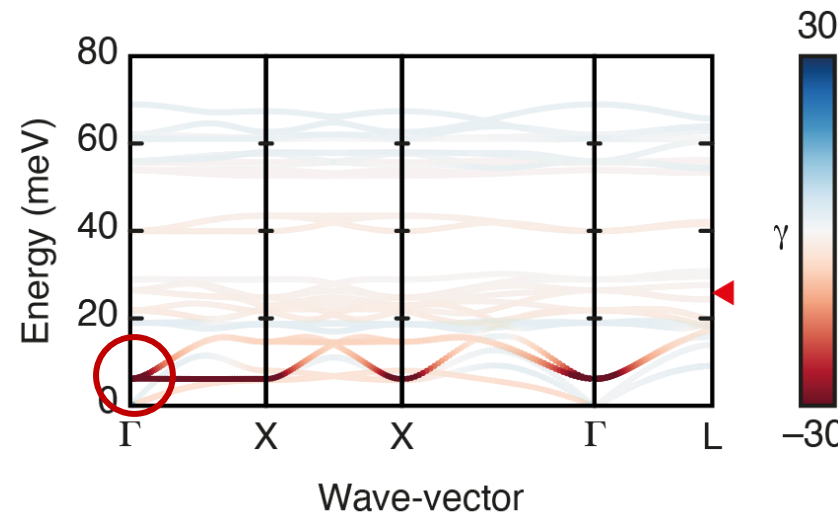
Correlated octahedral tilts



DFT calculations
 $\text{ZnPt}(\text{CN})_6$

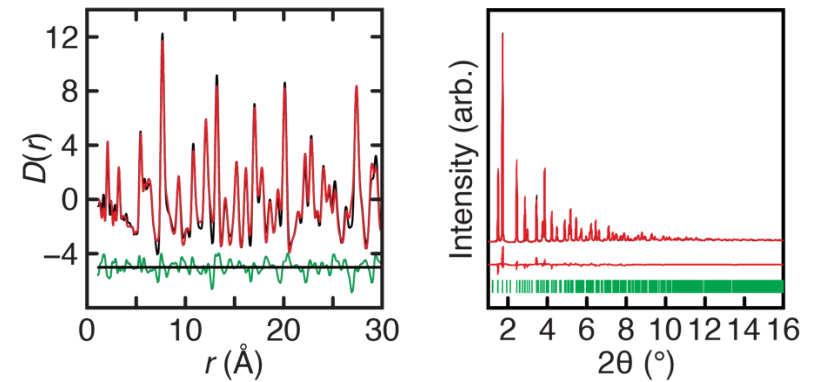


Empirical calculations
 $\text{MnPt}(\text{CN})_6$



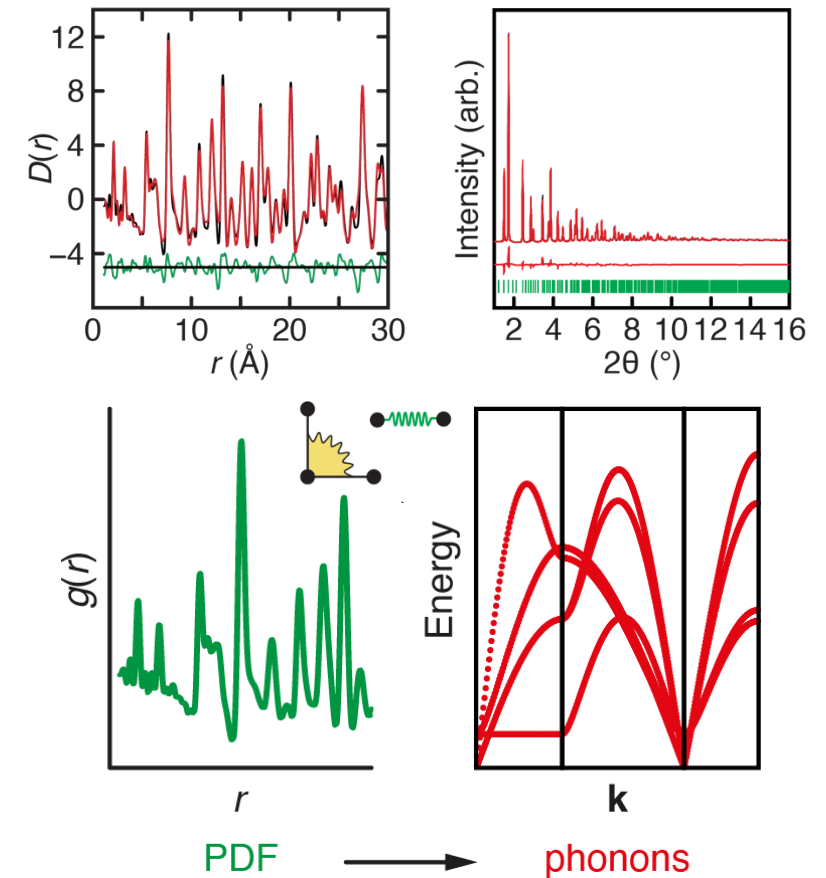
Conclusions

- **Simple model** — able to describe the **key thermal fluctuations**, accounting for both the **experimental PDF** and the intensities of **Bragg** reflections in the X-ray diffraction pattern.



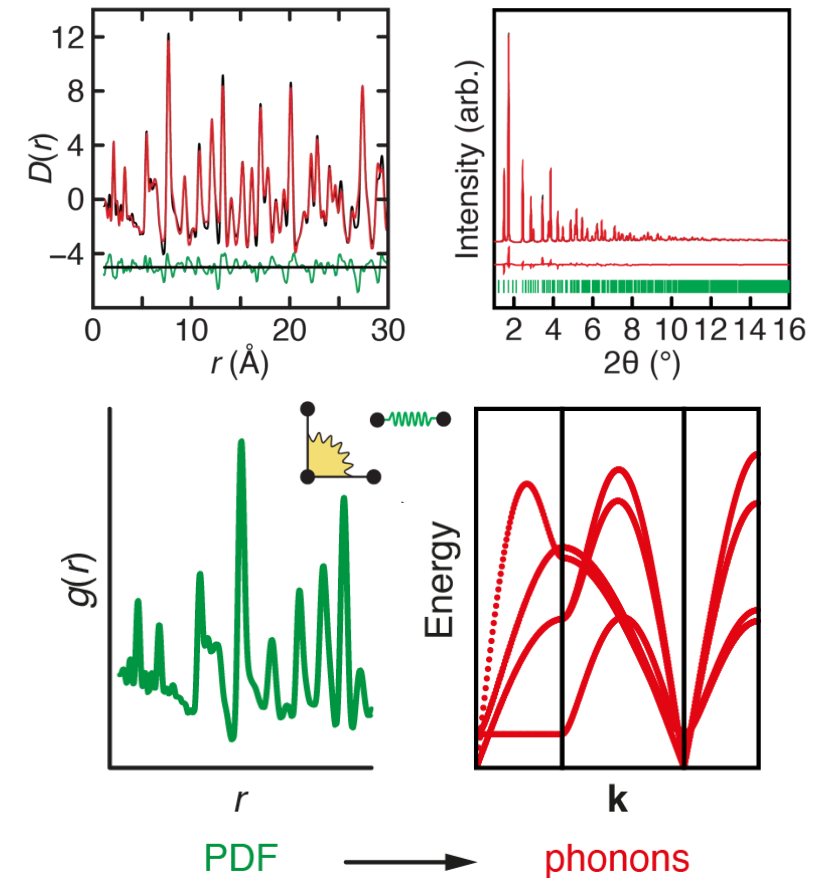
Conclusions

- **Simple model** — able to describe the **key thermal fluctuations**, accounting for both the **experimental PDF** and the intensities of **Bragg** reflections in the X-ray diffraction pattern.
- Sensitivity to pairwise correlations in these fluctuations — allows us to **interrogate** the **phonon dispersion relations** implicit in our empirical model.



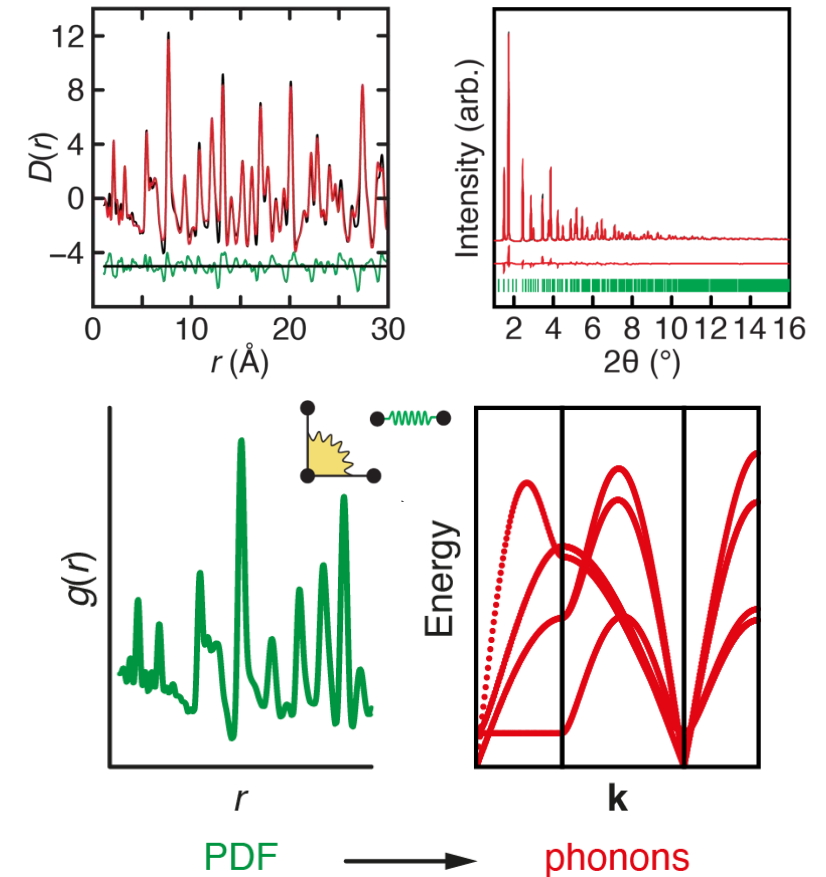
Conclusions

- **Simple model** — able to describe the **key thermal fluctuations**, accounting for both the **experimental PDF** and the intensities of **Bragg reflections** in the X-ray diffraction pattern.
- Sensitivity to pairwise correlations in these fluctuations — allows us to **interrogate the phonon dispersion relations** implicit in our empirical model.
- The **low-energy modes**, which dominate thermal motion and hence the variation in peak widths in the PDF, are surprisingly **well captured**.

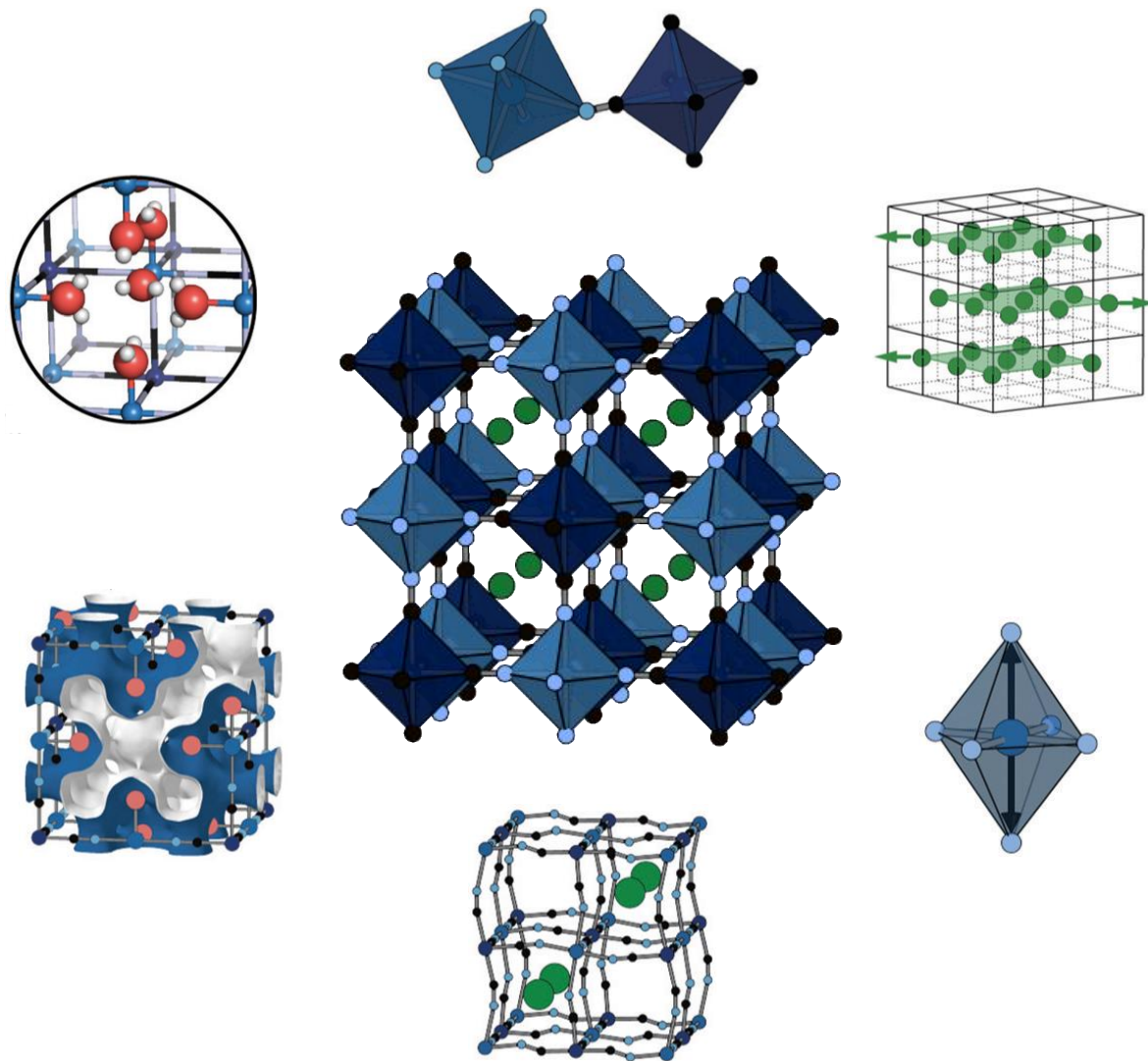


Conclusions

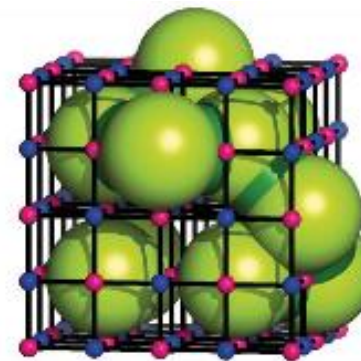
- **Simple model** — able to describe the **key thermal fluctuations**, accounting for both the **experimental PDF** and the intensities of **Bragg reflections** in the X-ray diffraction pattern.
- Sensitivity to pairwise correlations in these fluctuations — allows us to **interrogate the phonon dispersion relations** implicit in our empirical model.
- The **low-energy modes**, which dominate thermal motion and hence the variation in peak widths in the PDF, are surprisingly **well captured**.
- Able to identify the dominant NTE mechanism — **correlated octahedral tilts**.



Structural complexity in PBAs

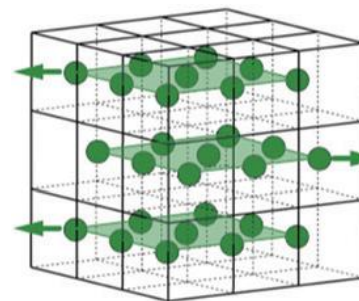


J. Cattermull, M. Pasta, A. L. Goodwin, *Mater. Horiz.*, **2021**, 8, 3178



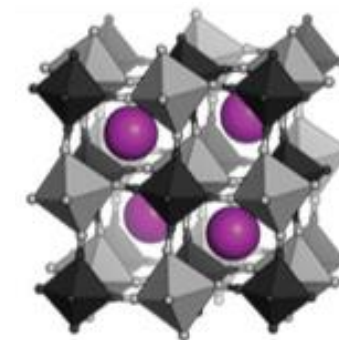
Correlated vacancies

Simonov *et al*,
Nature **2020**,
578, 256



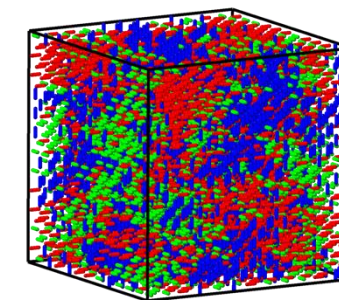
A-site 'slides'

Cattermull *et al*,
JACS **2023**, 145,
24249



Octahedral tilts

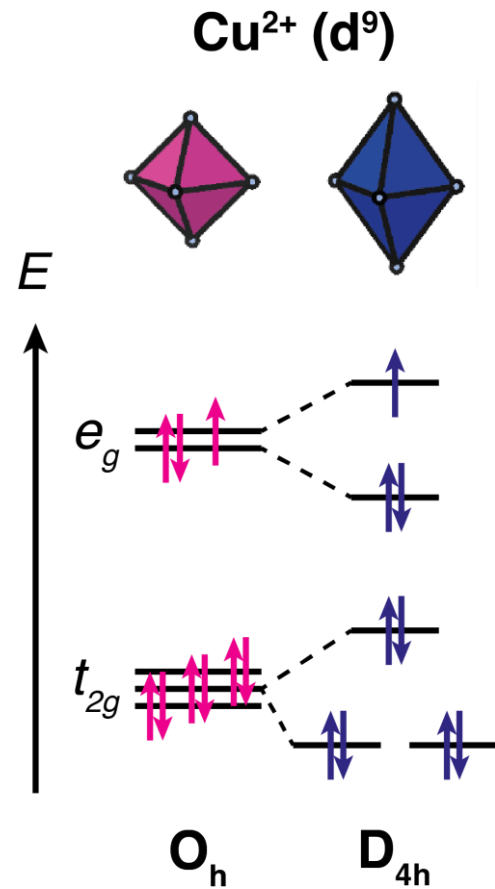
Boström & Brant,
J. Mater. Chem. C.
2022, 10, 13690



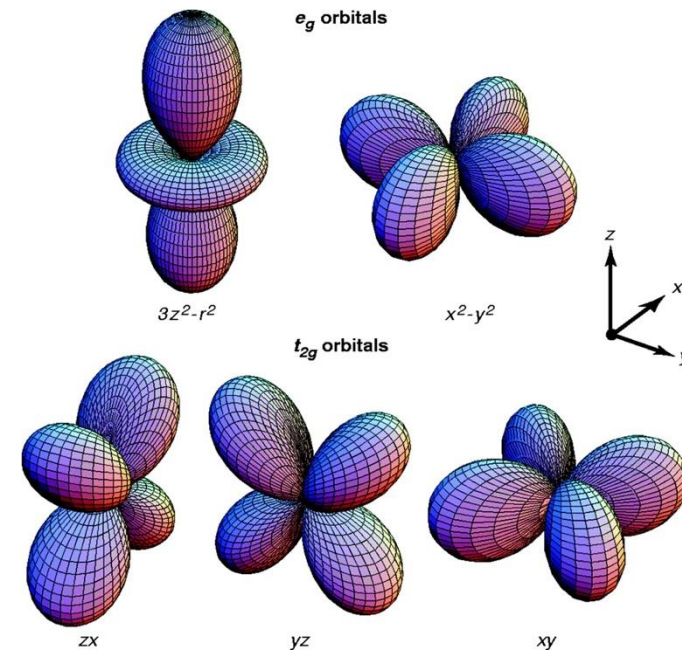
Cooperative JT

Harbourne *et al*
arXiv:2408.13169
2024

Jahn–Teller

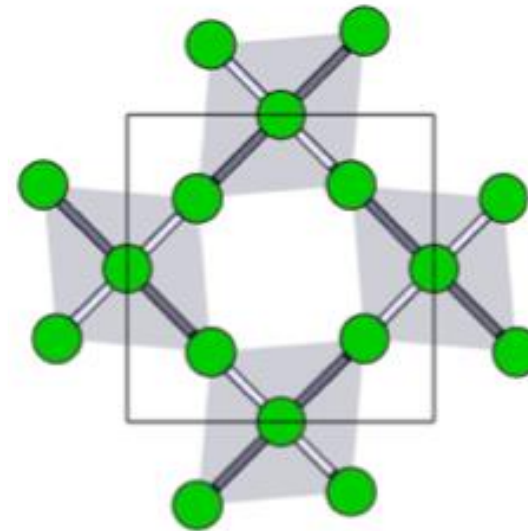
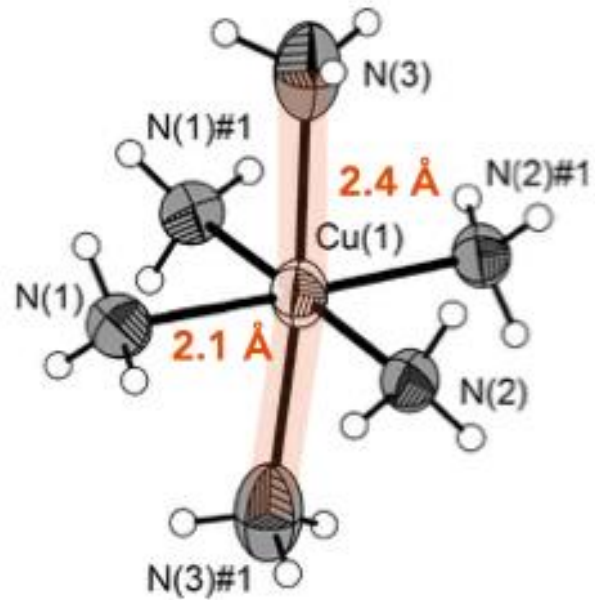


Jahn & Teller,
Proc. R. Soc. Lond. A.,
1937, 161, 220



Y. Tokura & N. Nagaosa,
Science **2000**, 288, 462

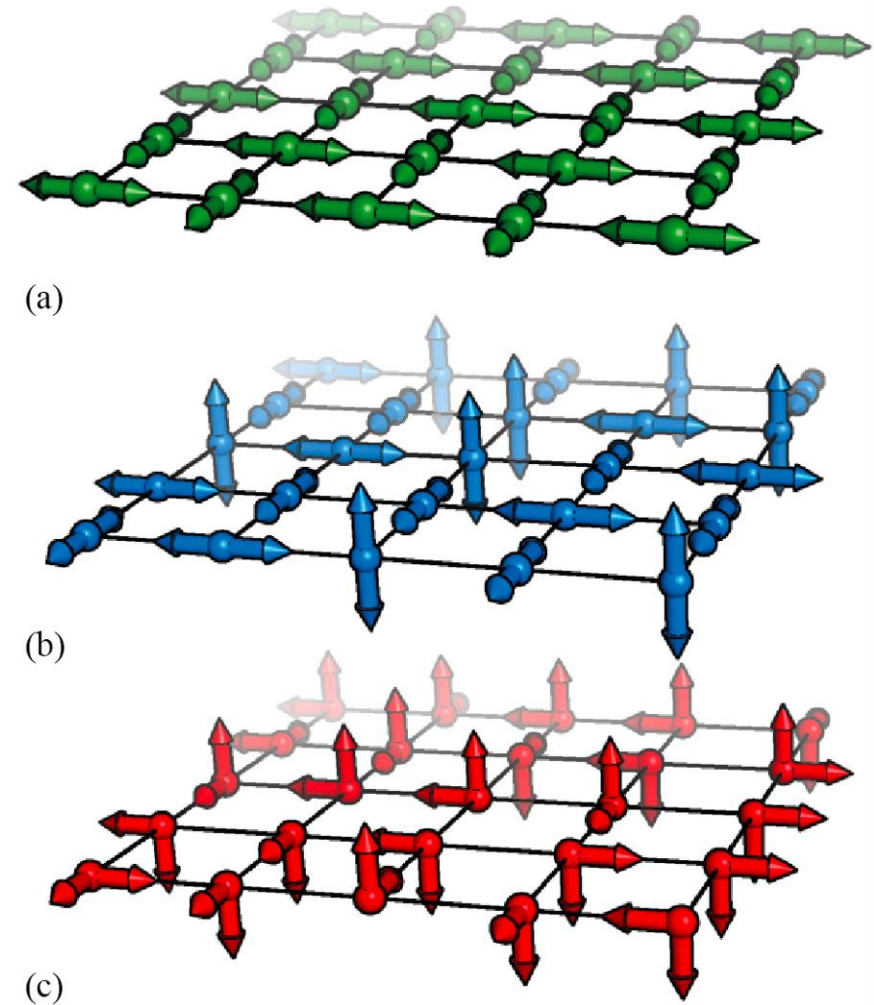
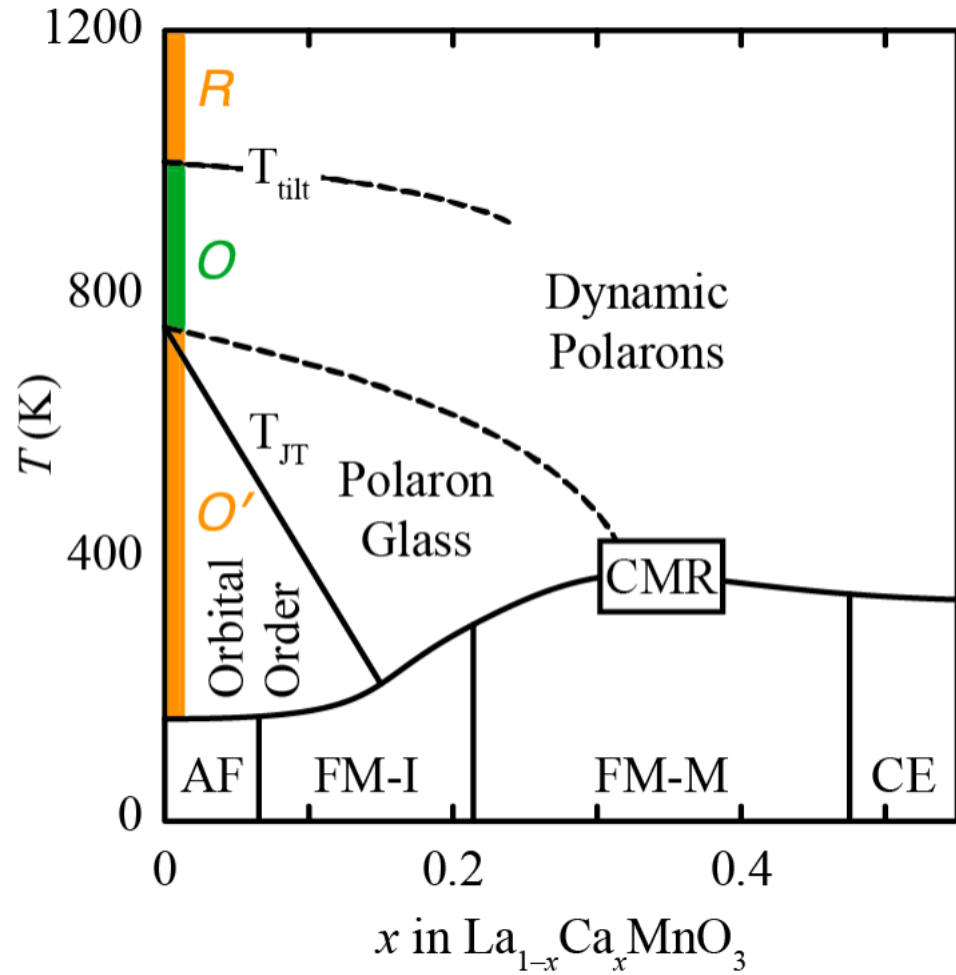
Jahn–Teller



Woidy, Meng & Kraus, *Z. Naturforsch B.* **2014**, 69, 1

Okazaki & Suemune, *J. Phys. Soc. Jpn.* **1961**, 16, 176

Cooperative JT order/disorder: LCMO

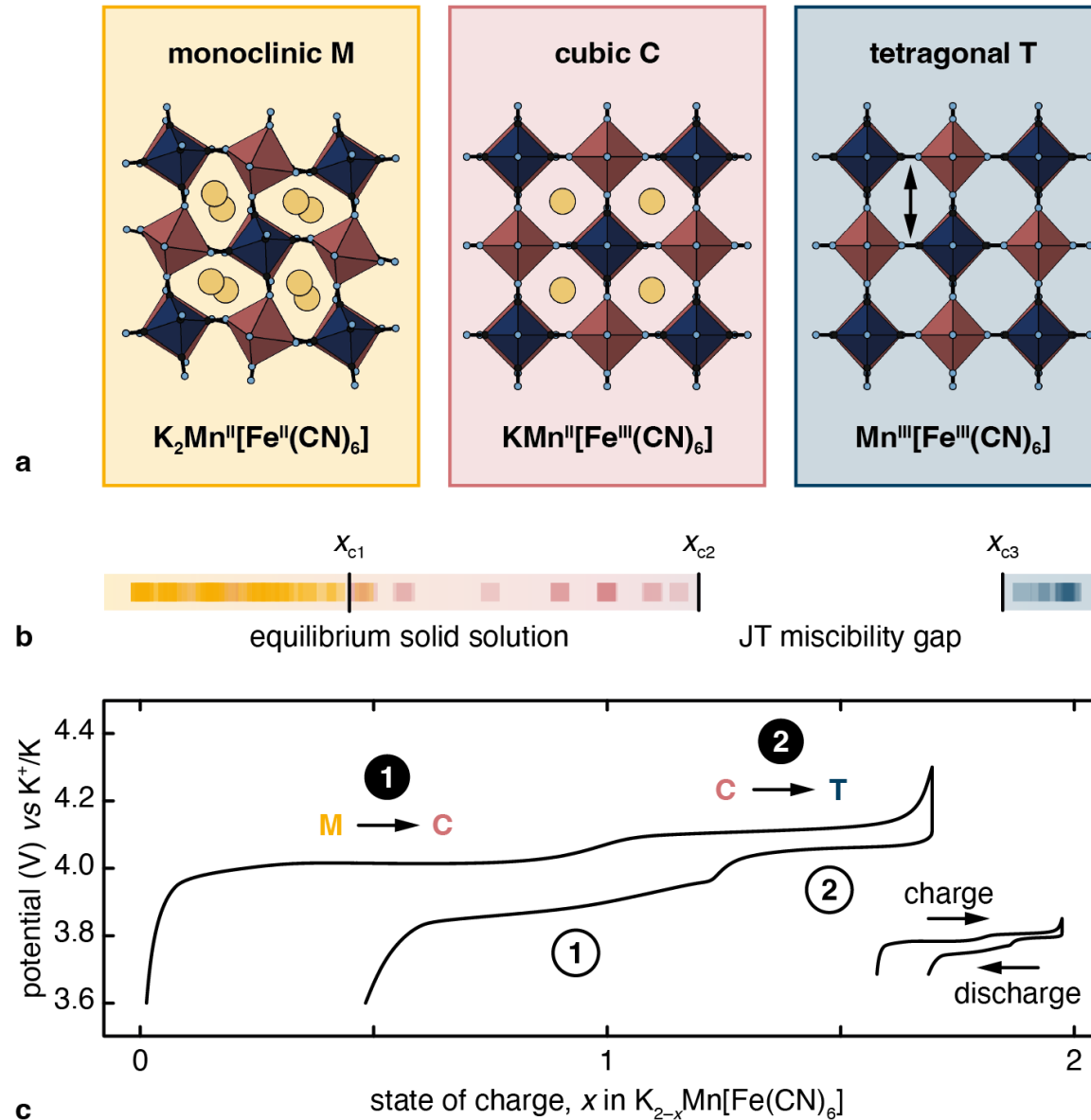


Jin, Tiefel, McCormack, Fastnacht, Ramesh and Chen, *Science* **1994**, 264, 413

Thygesen, Young, Beake, Romero, Connor, Proffen, Phillips, Tucker, Hayward, Keen and Goodwin, *Phys. Rev. B* **2017**, 95, 174107

PBA K-ion cathode materials

Cattermull, Jagger,
Cassidy, Dhir, Allan,
Pasta, Goodwin,
arXiv: 2509.04587

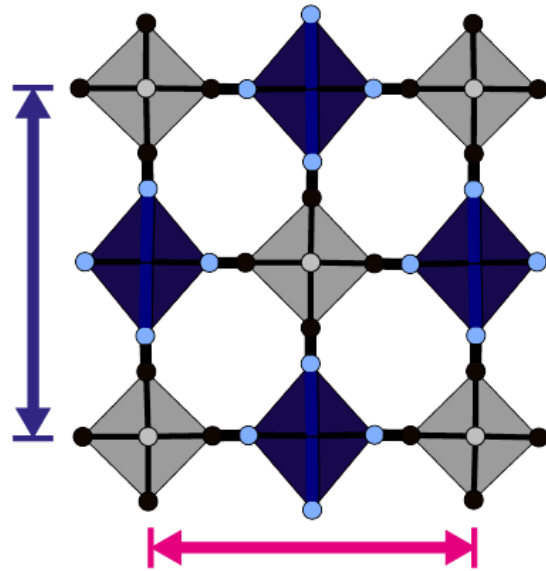


Wessells, Huggins, Cui,
Nat. Commun., **2011**, 2, 550

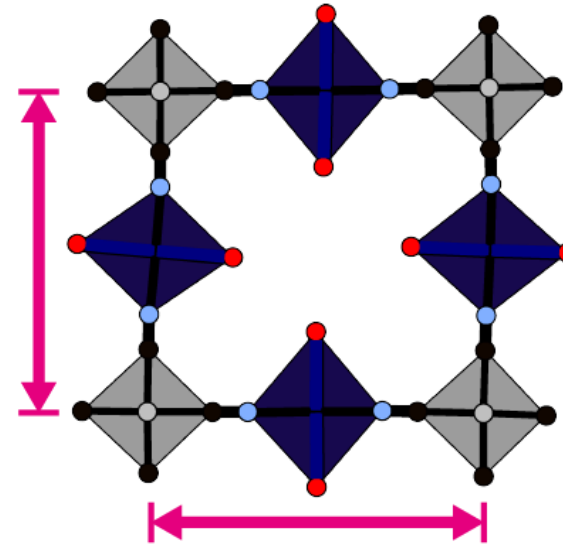
Deng, Qu, Niu, Liu, Zhang, Hong,
Feng, Wang, Hu, Zeng, Zhang,
Guo, Zhu,
Nat. Commun., **2021**, 12, 2167

Solution?

Exploit the **interplay** of **JT** concentration, **vacancy** concentration, and long-range symmetry breaking

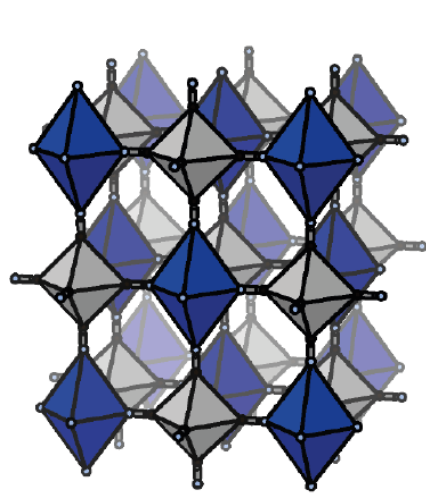


tetragonal
 $\text{Cu}[\text{Pt}(\text{CN})_6]$

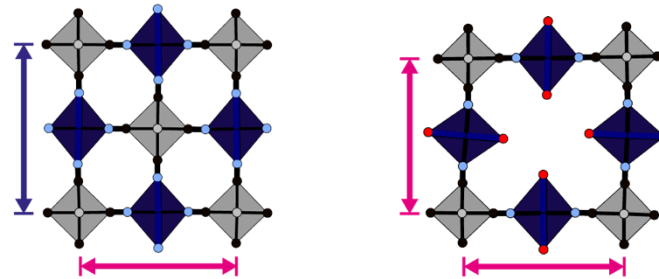
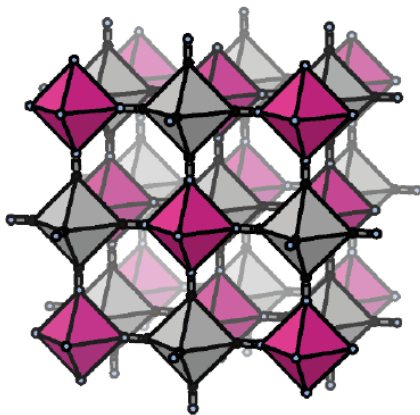


cubic
 $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$

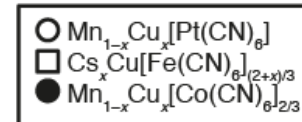
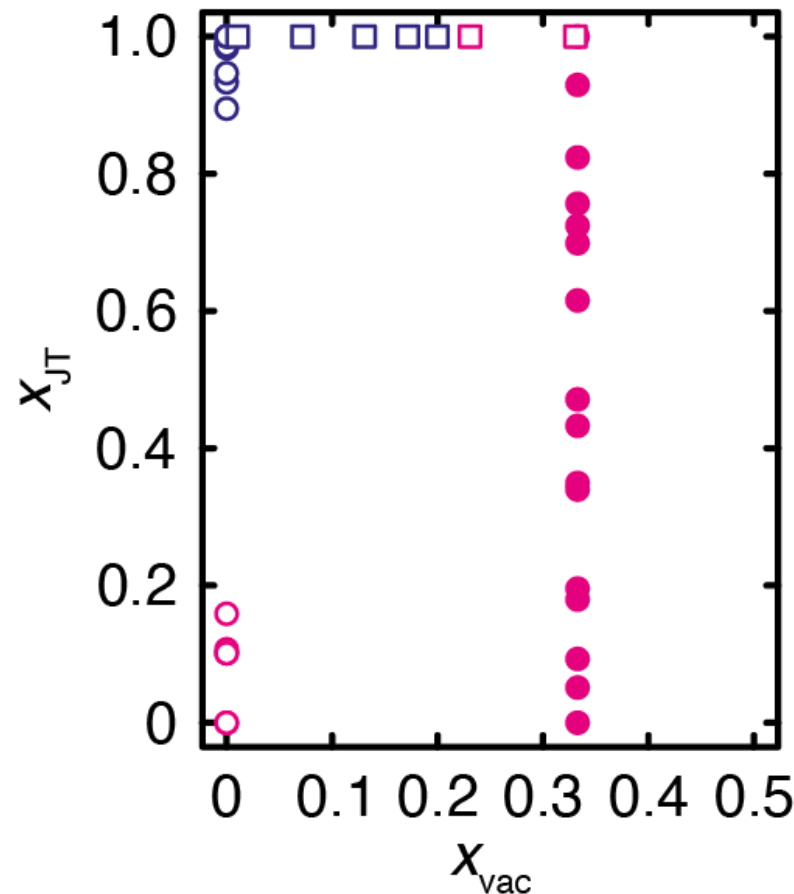
Phase map – interplay of JT/vacancy concentration



$(\text{Cu}_x\text{Mn}_{1-x})[\text{Pt}(\text{CN})_6]$
no vacancies,
varying JT

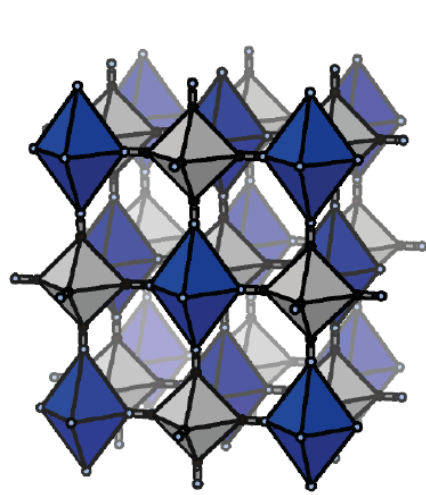


$\text{Cs}_{1-3x_{\text{vac}}}\text{Cu}[\text{Fe}(\text{CN})_6]_{1-x_{\text{vac}}}$
max JT, varying vacancies

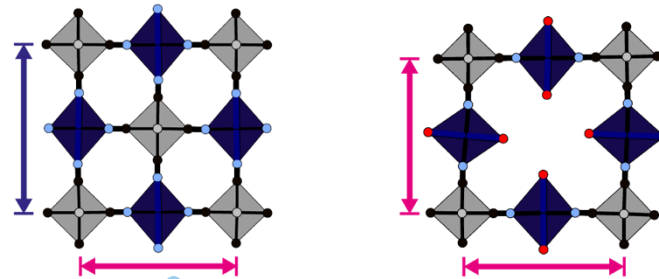
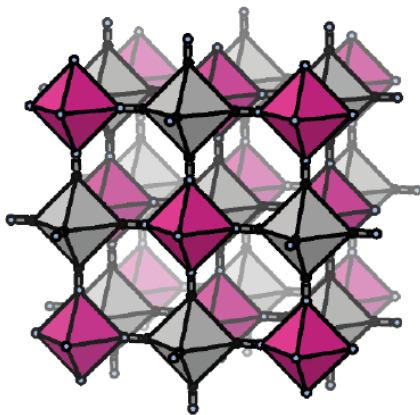


$(\text{Cu}_x\text{Mn}_{1-x})[\text{Co}(\text{CN})_6]_{2/3}$
max vacancies, varying JT

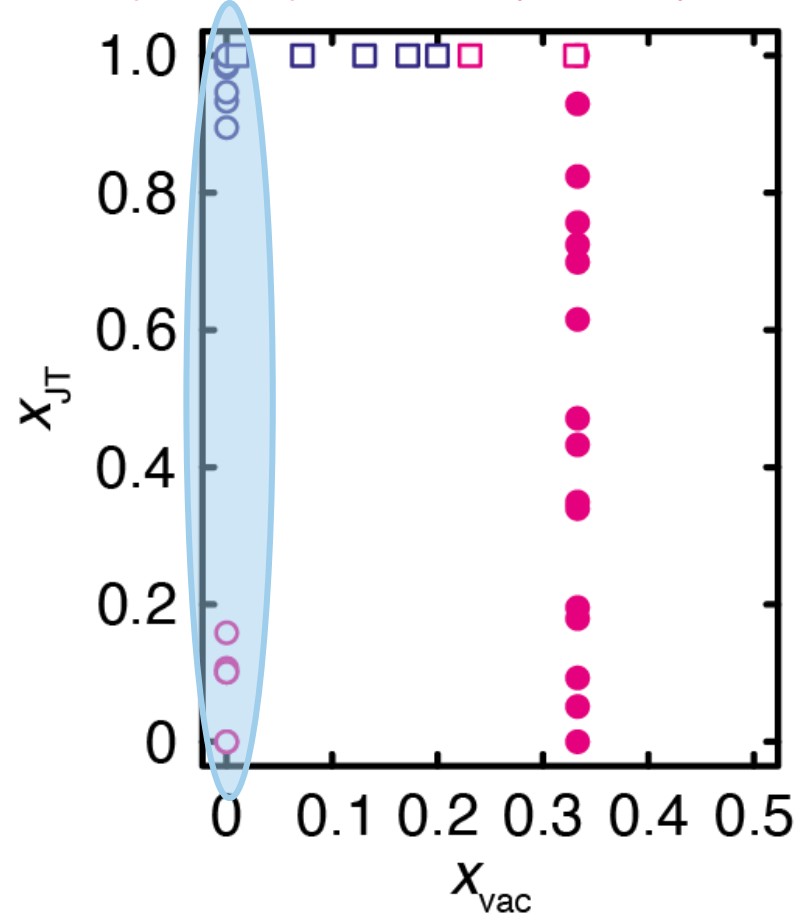
Phase map – interplay of JT/vacancy concentration



$(\text{Cu}_x\text{Mn}_{1-x})[\text{Pt}(\text{CN})_6]$
no vacancies,
varying JT

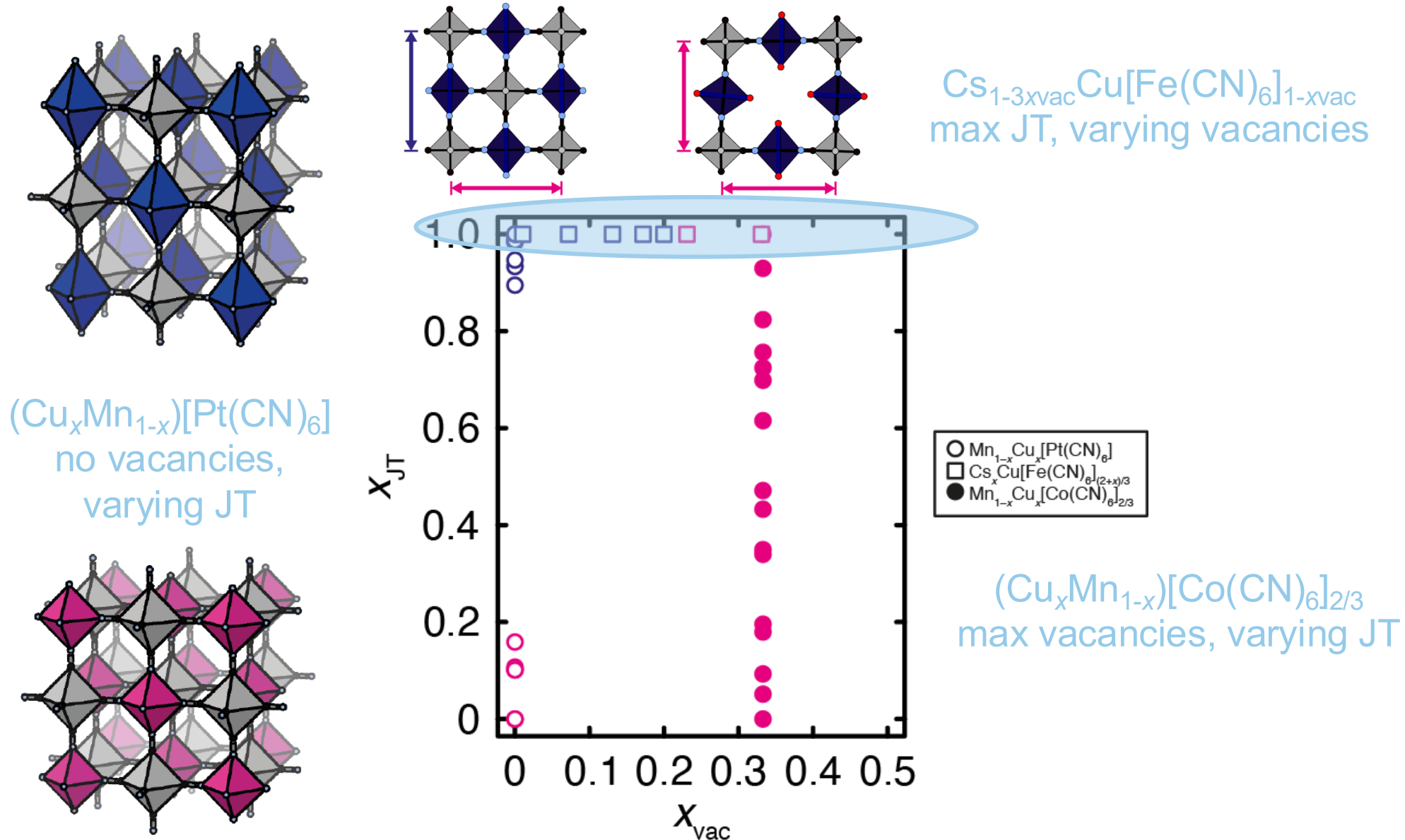


$\text{Cs}_{1-3x_{\text{vac}}}\text{Cu}[\text{Fe}(\text{CN})_6]_{1-x_{\text{vac}}}$
max JT, varying vacancies

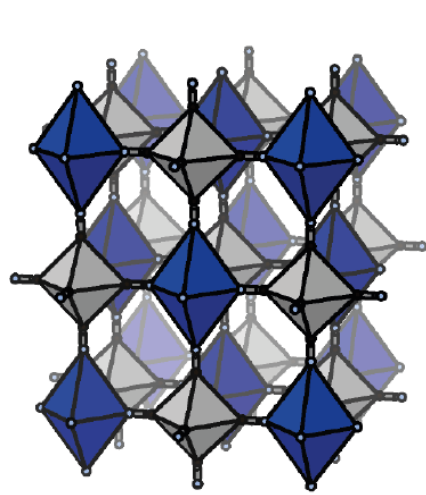


$(\text{Cu}_x\text{Mn}_{1-x})[\text{Co}(\text{CN})_6]_{2/3}$
max vacancies, varying JT

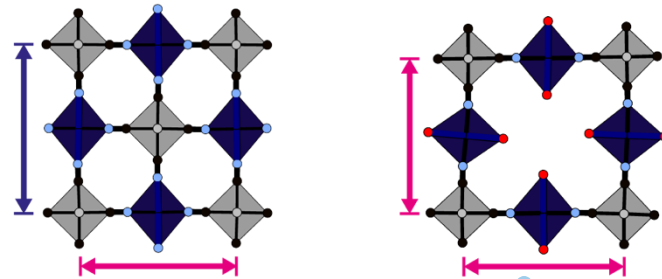
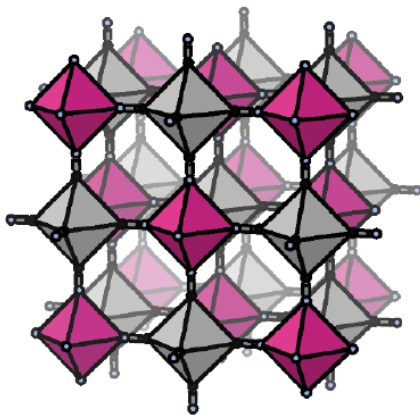
Phase map – interplay of JT/vacancy concentration



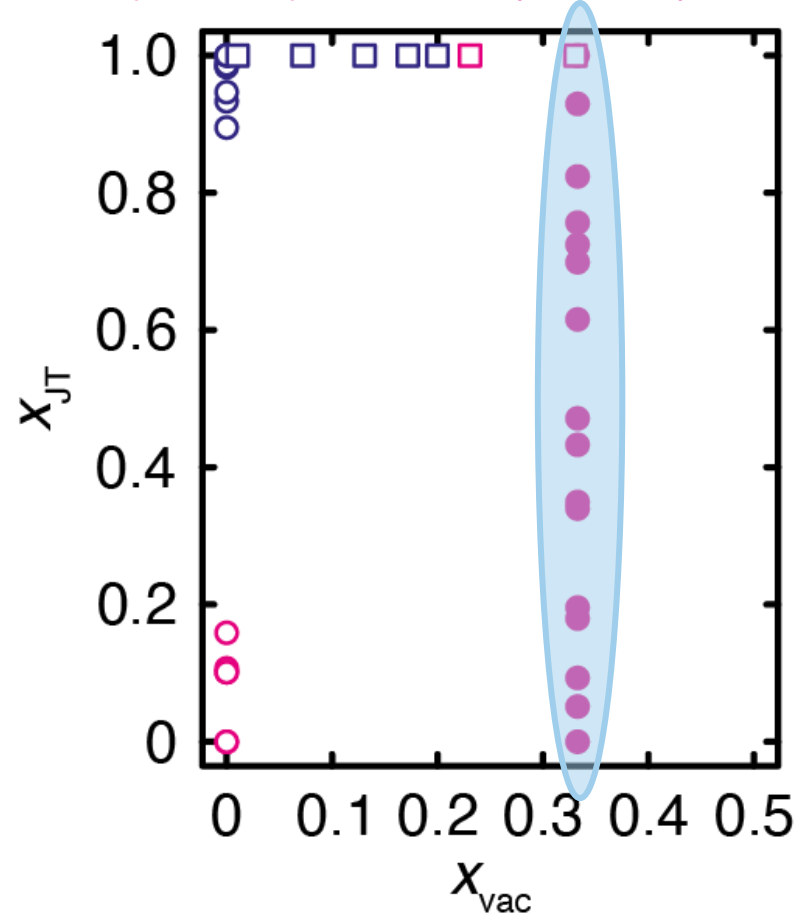
Phase map – interplay of JT/vacancy concentration



$(\text{Cu}_x\text{Mn}_{1-x})[\text{Pt}(\text{CN})_6]$
no vacancies,
varying JT

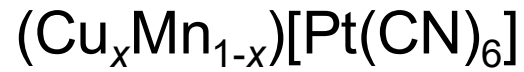


$\text{Cs}_{1-3x_{\text{vac}}}\text{Cu}[\text{Fe}(\text{CN})_6]_{1-x_{\text{vac}}}$
max JT, varying vacancies

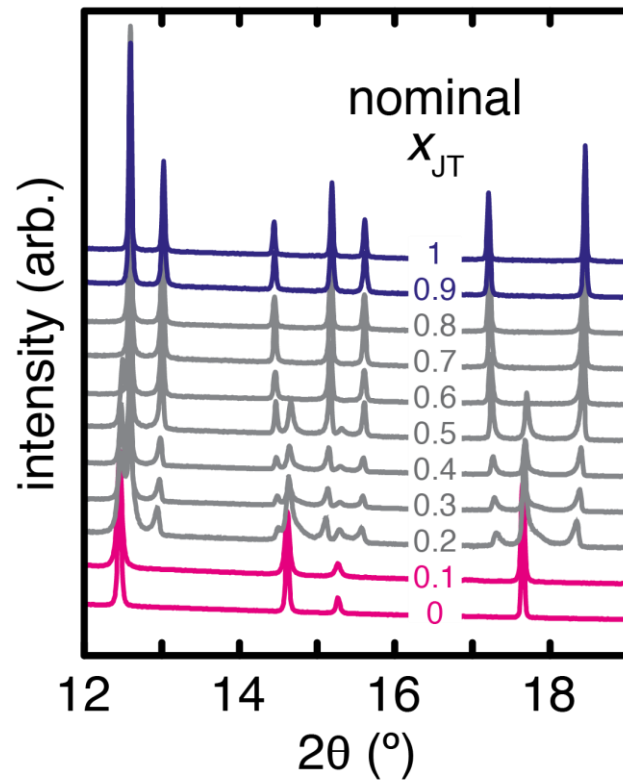


$(\text{Cu}_x\text{Mn}_{1-x})[\text{Co}(\text{CN})_6]_{2/3}$
max vacancies, varying JT

$(\text{Cu}_x\text{Mn}_{1-x})[\text{Pt}(\text{CN})_6]$ – no vacancies, vary JT

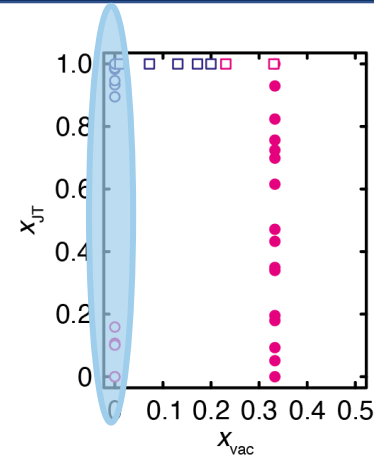
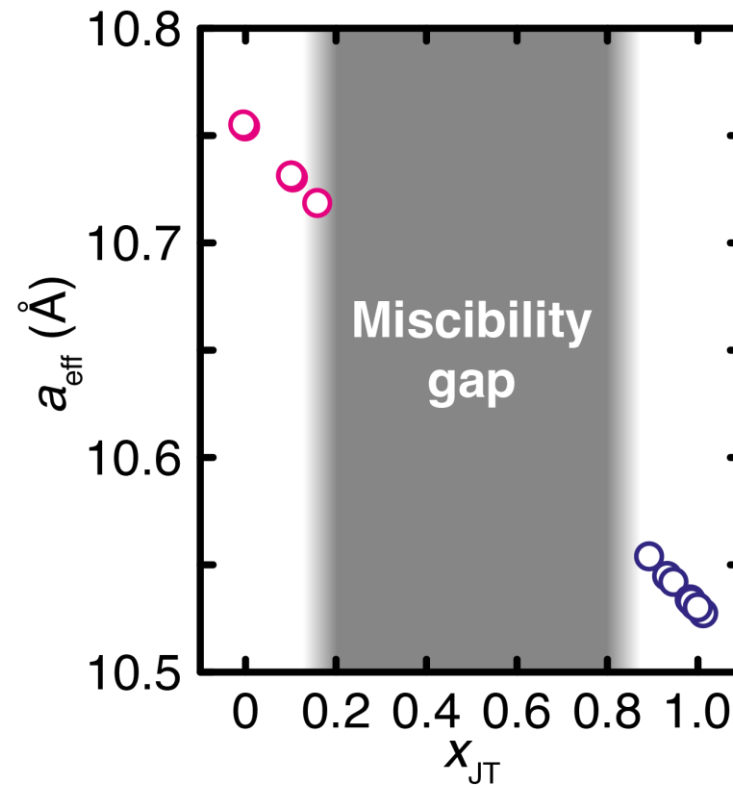


vary x_{JT} , $x_{\text{vac}} = 0$



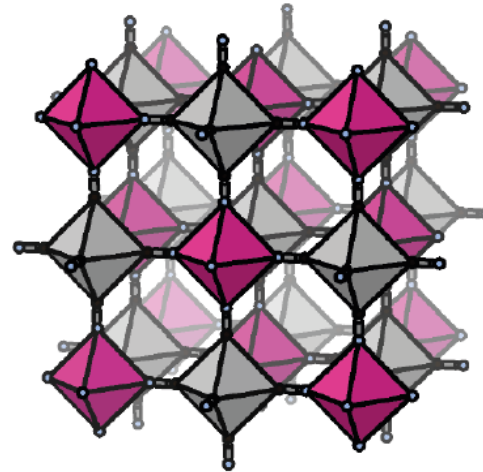
max JT: $\text{Cu}[\text{Pt}(\text{CN})_6]$ is tetragonal

min JT: $\text{Mn}[\text{Pt}(\text{CN})_6]$ is cubic

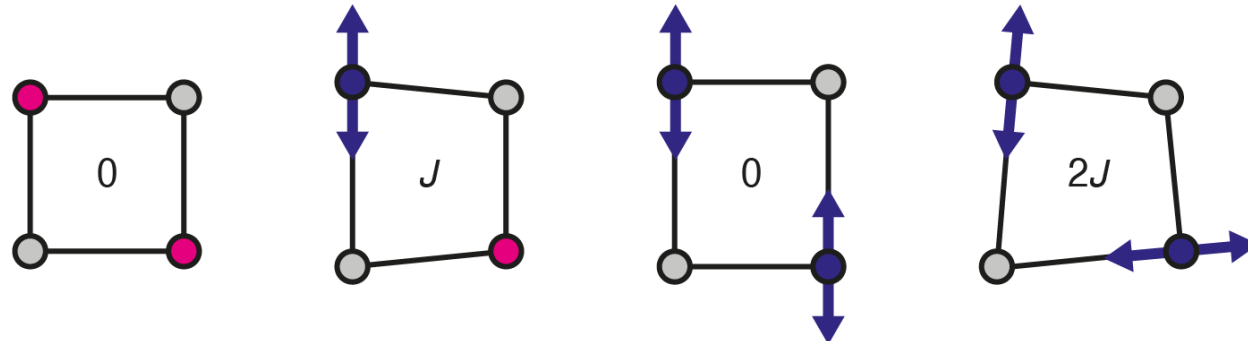
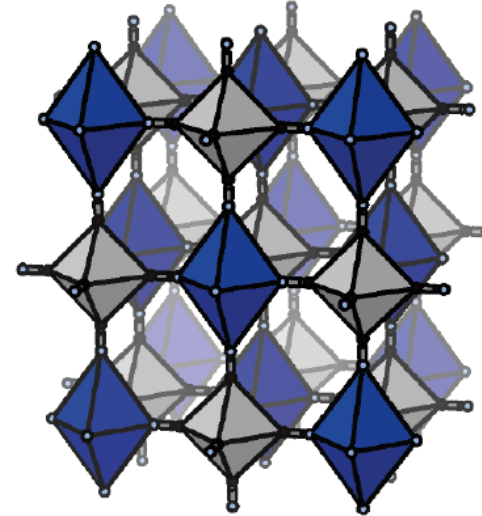


Strain coupling in PBAs

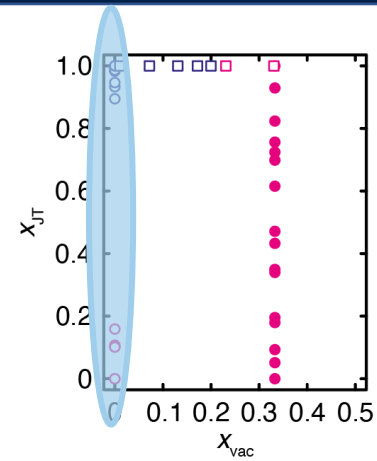
Mn[Pt(CN)₆]



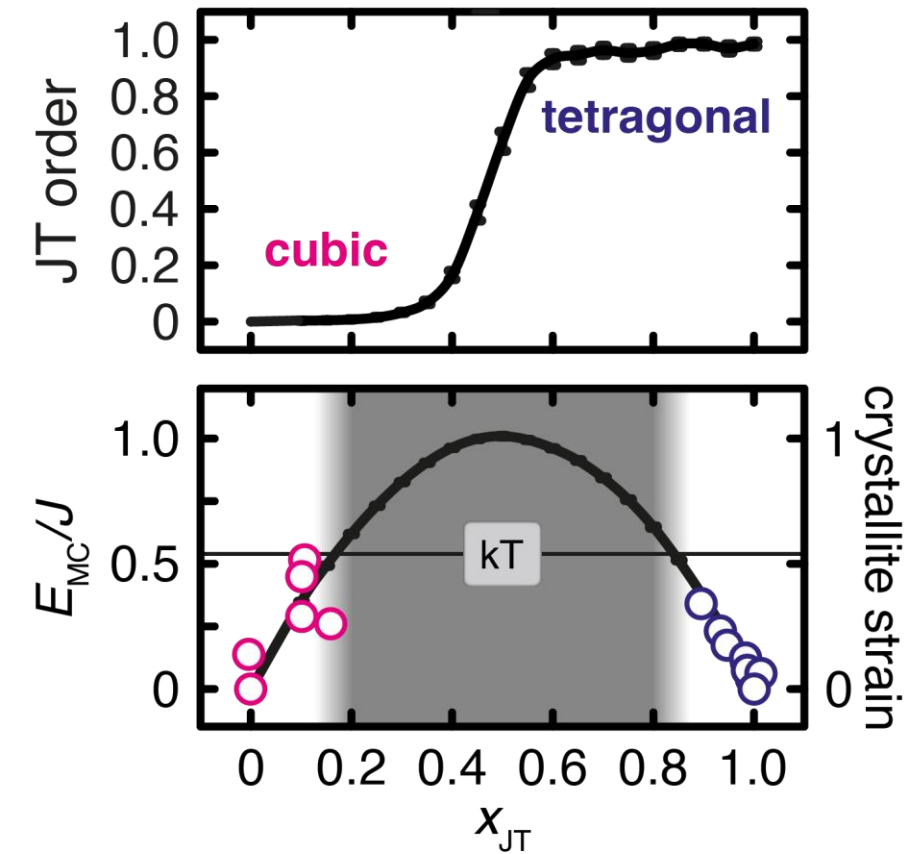
Cu[Pt(CN)₆]



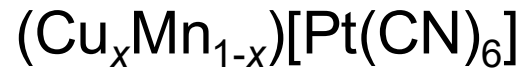
angle **strain**
Monte Carlo



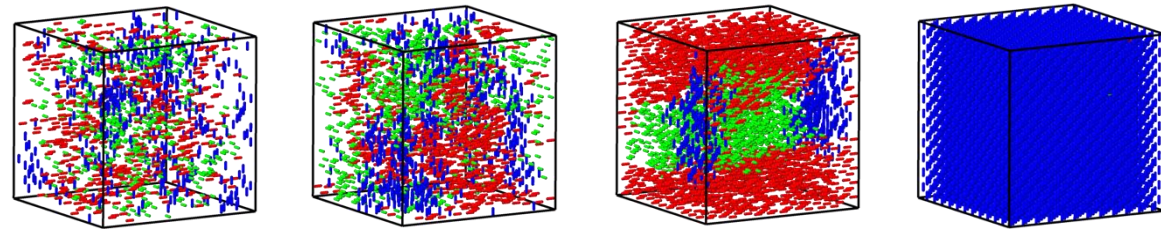
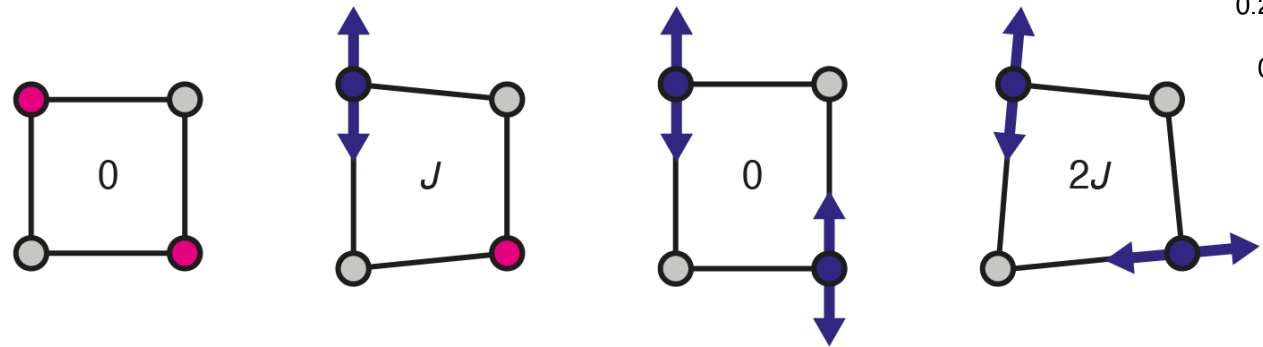
$(\text{Cu}_x\text{Mn}_{1-x})[\text{Pt}(\text{CN})_6]$ – no vacancies, vary JT



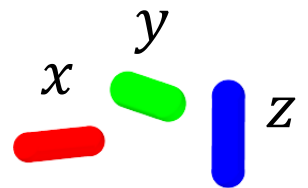
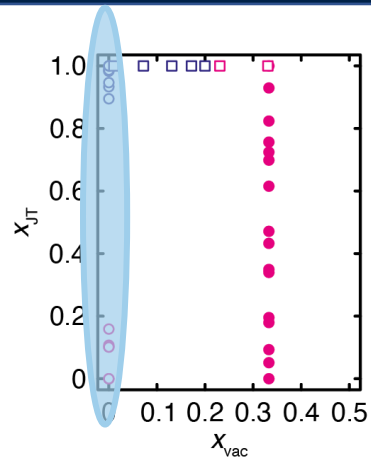
J captures strain
energy scale
 $\sim 5 \text{ kJ mol}^{-1}$



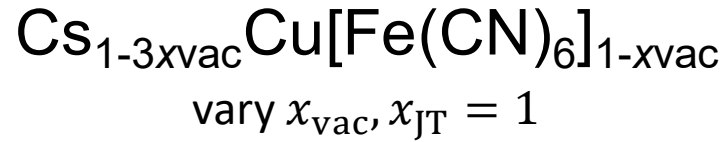
vary x_{JT} , $x_{\text{vac}} = 0$



$x_{\text{JT}} = 0.2$ $x_{\text{JT}} = 0.3$ $x_{\text{JT}} = 0.5$ $x_{\text{JT}} = 1$



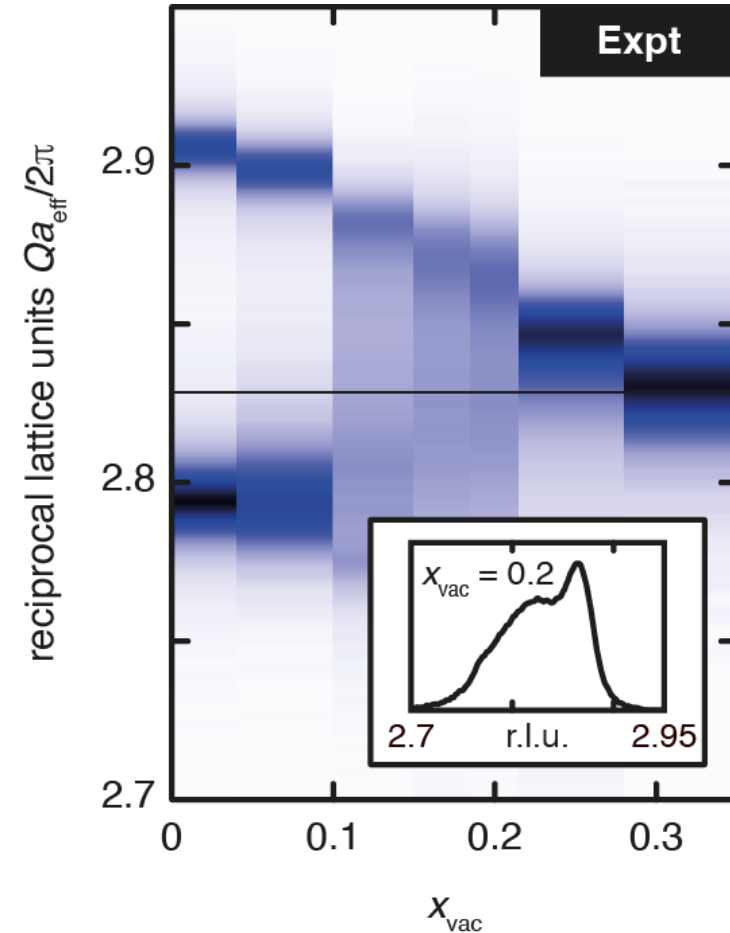
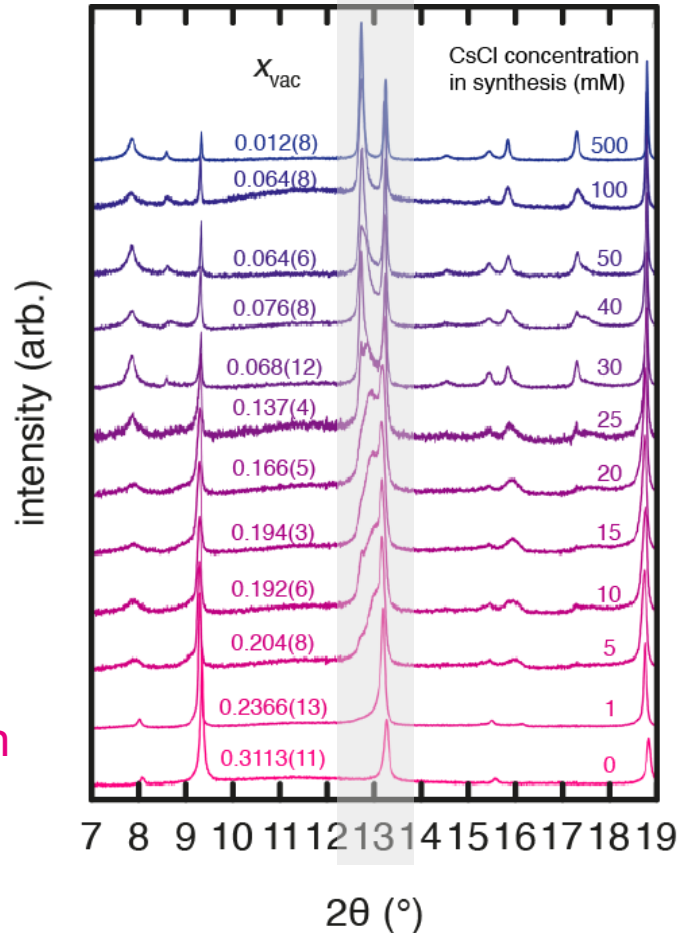
$\text{Cs}_{1-3x_{\text{vac}}}\text{Cu}[\text{Fe}(\text{CN})_6]_{1-x_{\text{vac}}}$: max JT, varying vacancies



vacancy-free
 $\text{CsCu}[\text{Fe}(\text{CN})_6]$ is
tetragonal

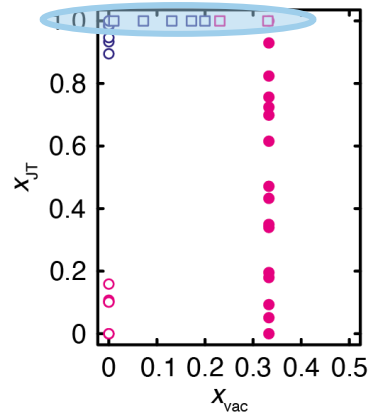
increasing
 $[\text{Fe}(\text{CN})_6]^{3-}$
vacancy
fraction

Limiting composition
 $\text{Cu}[\text{Fe}(\text{CN})_6]_{2/3}$ is
cubic



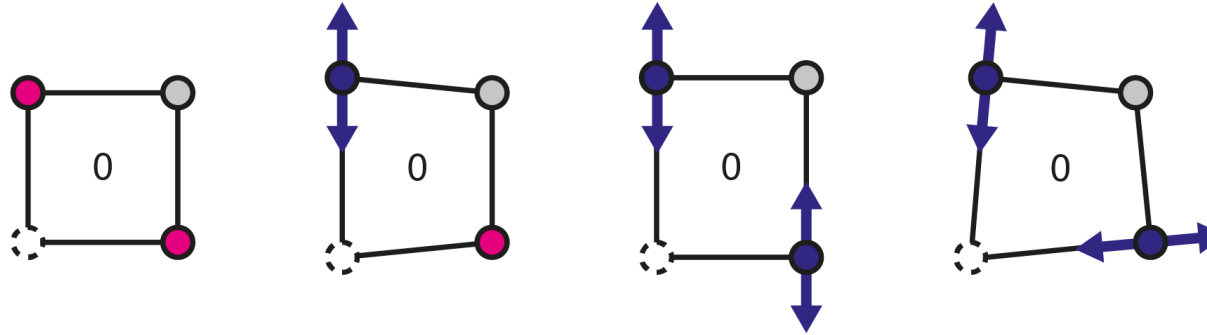
{220} position

critical
 $x_{\text{vac}} \approx 0.2$

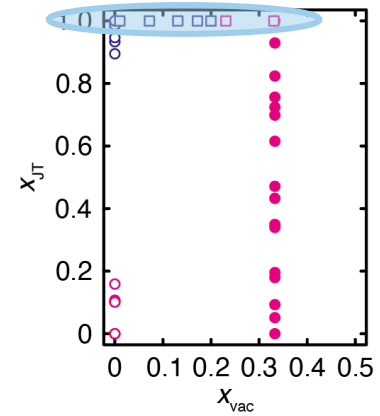


Vacancy-driven cooperative JT melting

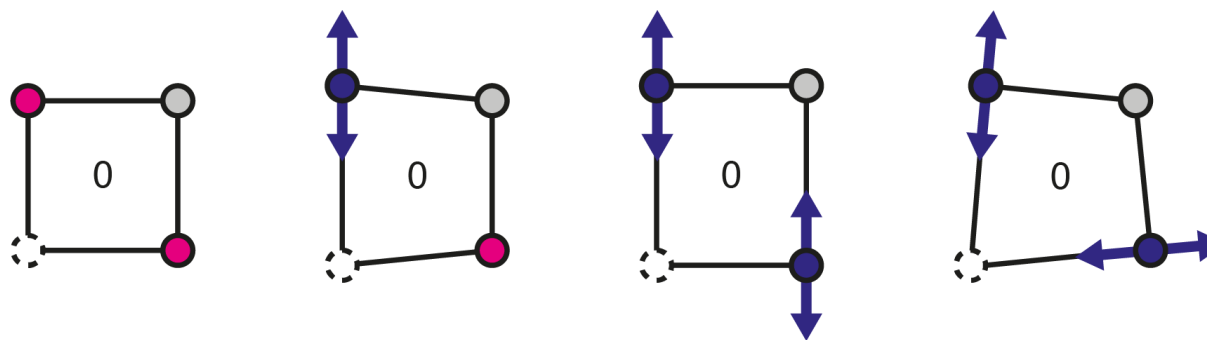
Vacancy incorporation



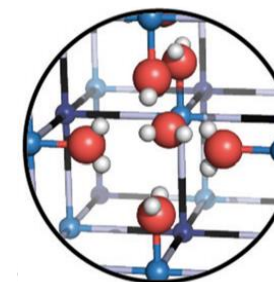
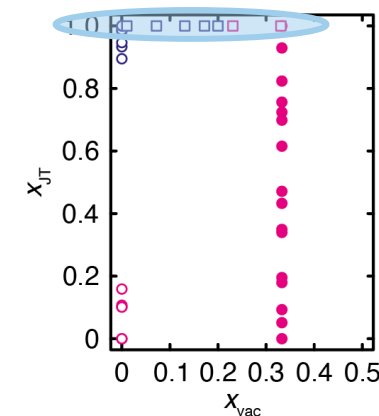
vacancy relieves all angular strain



Vacancy incorporation



vacancy relieves all angular strain



JT-distortion prefers
to **point towards a
vacancy**/be capped
with OH₂

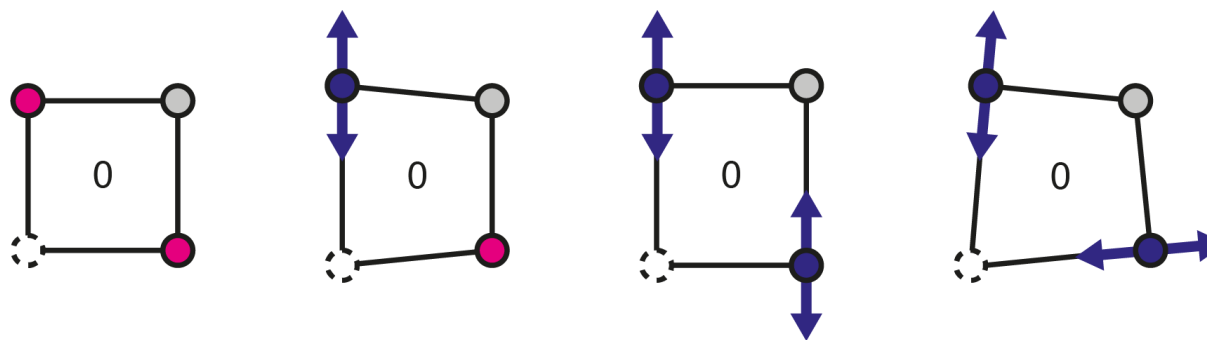
DFT study of copper
hexacyanoferrates:

X. Wang, A. T. Ta, S. Quemerais, A.

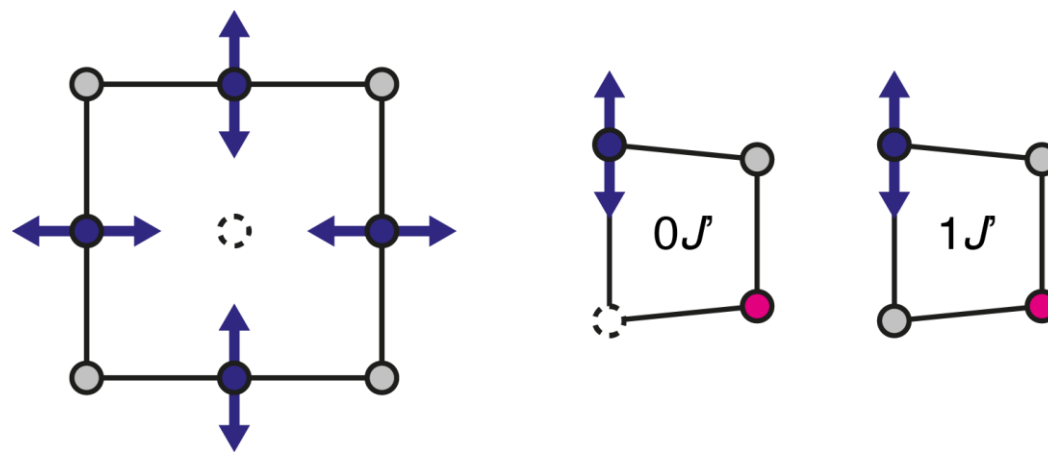
Grandjean, H.-C. zur Loye, S. R.

Phillpot, *Chem. Mater.*, **2024**, 36, 6731

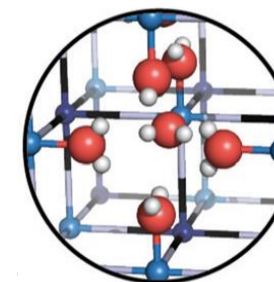
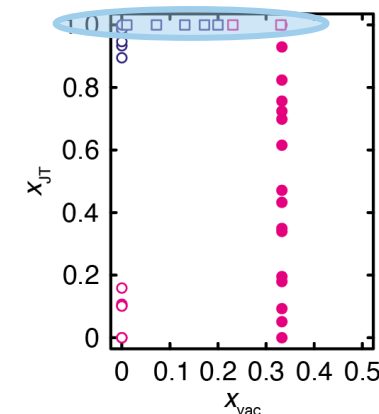
Vacancy incorporation



vacancy relieves all angular strain



crystal-field preference



JT-distortion prefers to **point towards a vacancy**/be capped with OH_2

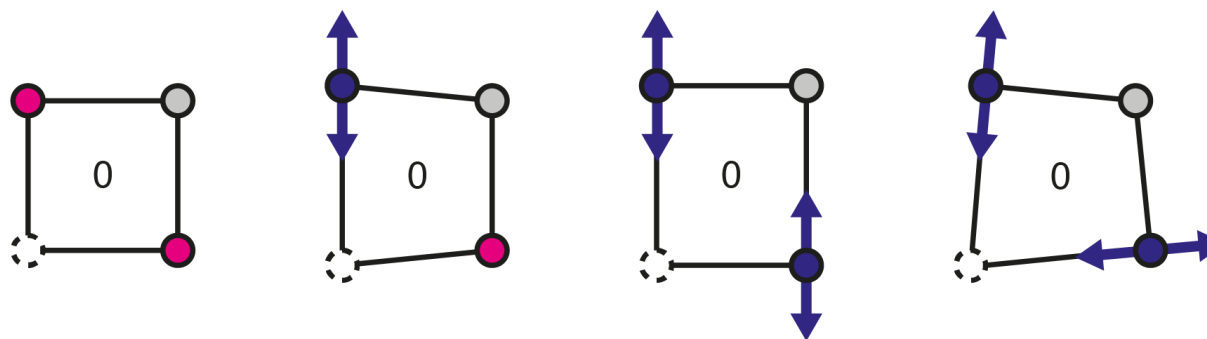
DFT study of copper hexacyanoferrates:

X. Wang, A. T. Ta, S. Quemerais, A.

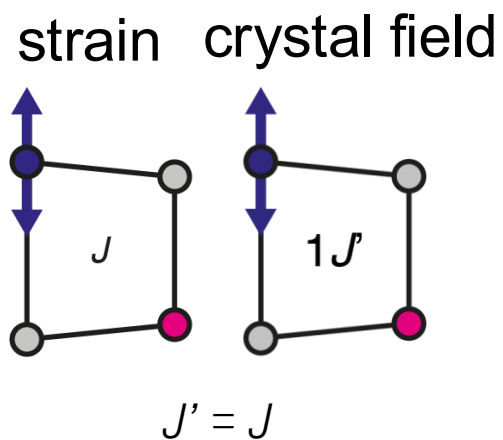
Grandjean, H.-C. zur Loye, S. R.

Phillpot, *Chem. Mater.*, **2024**, 36, 6731

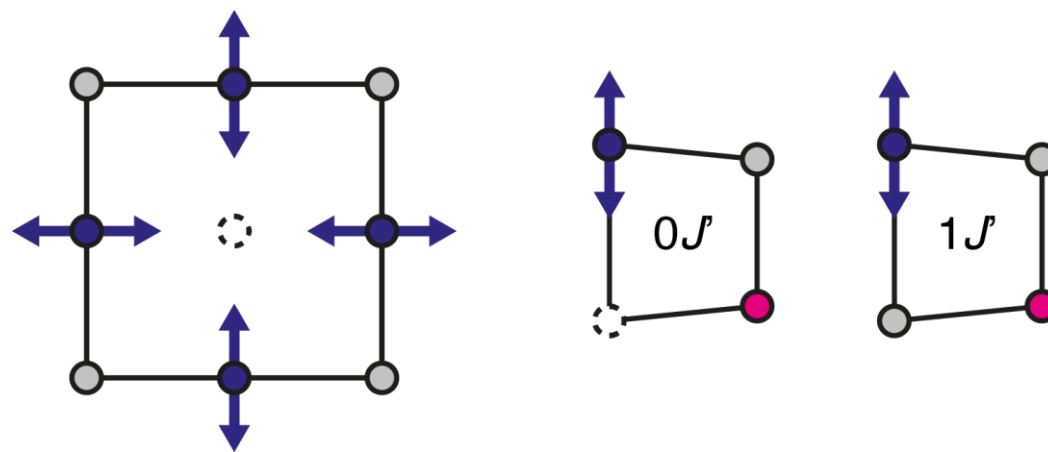
Vacancy incorporation



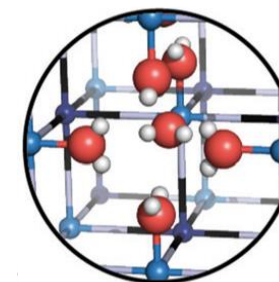
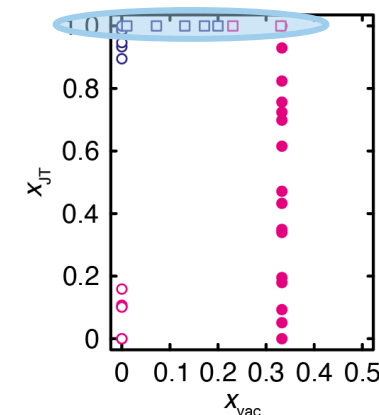
vacancy relieves all angular strain



J' different for different systems



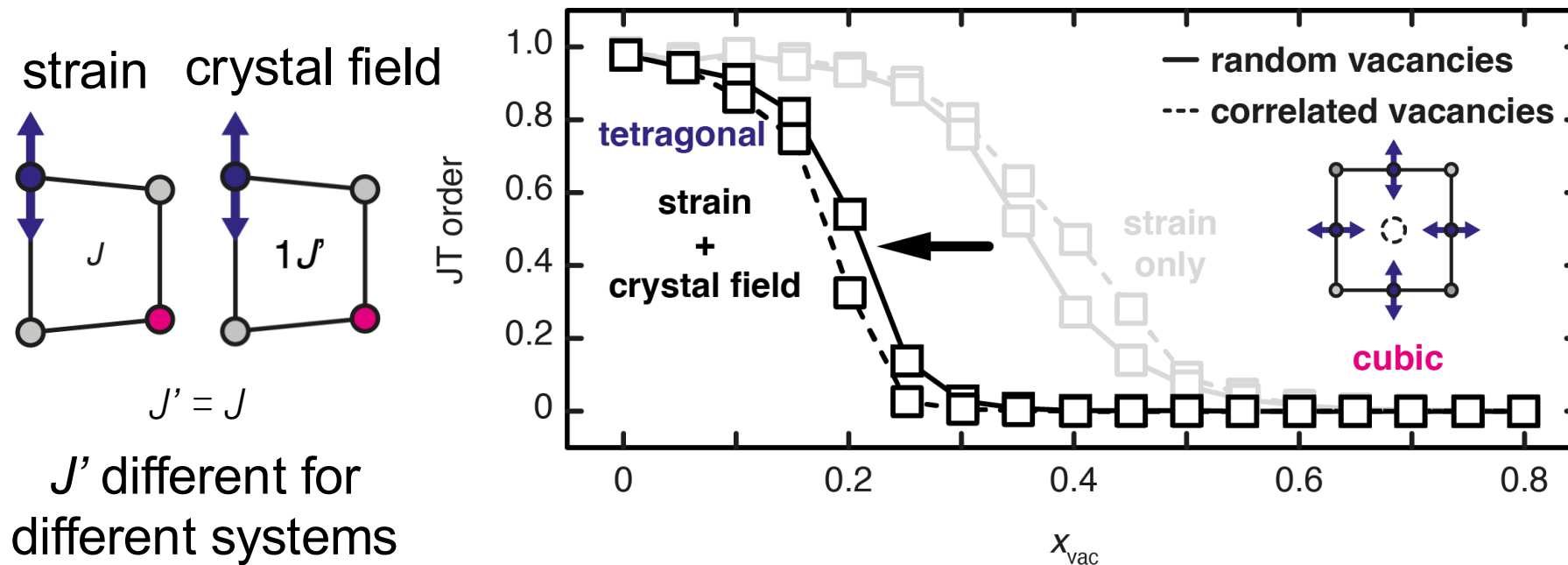
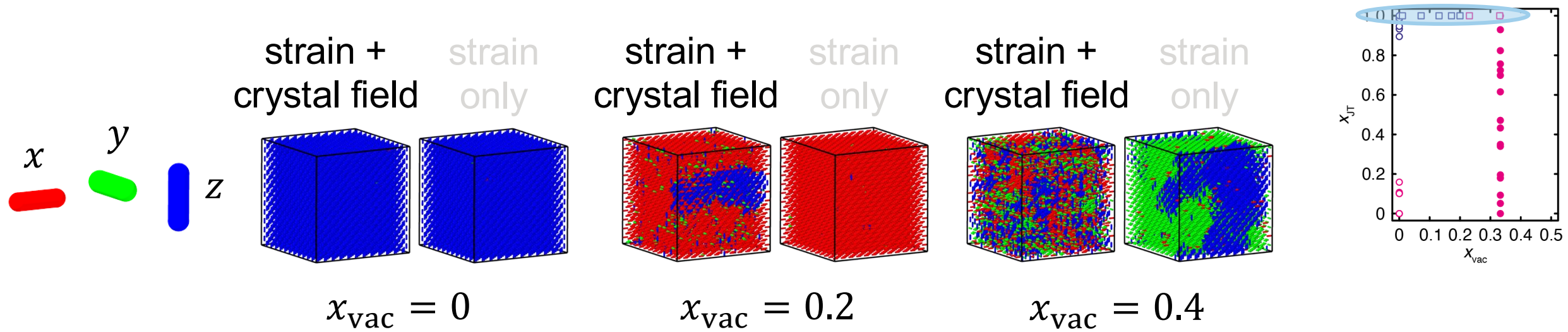
crystal-field preference



JT-distortion prefers to **point towards a vacancy**/be capped with OH_2

DFT study of copper hexacyanoferrates:
X. Wang, A. T. Ta, S. Quemerais, A. Grandjean, H.-C. zur Loye, S. R. Phillpot, *Chem. Mater.*, **2024**, 36, 6731

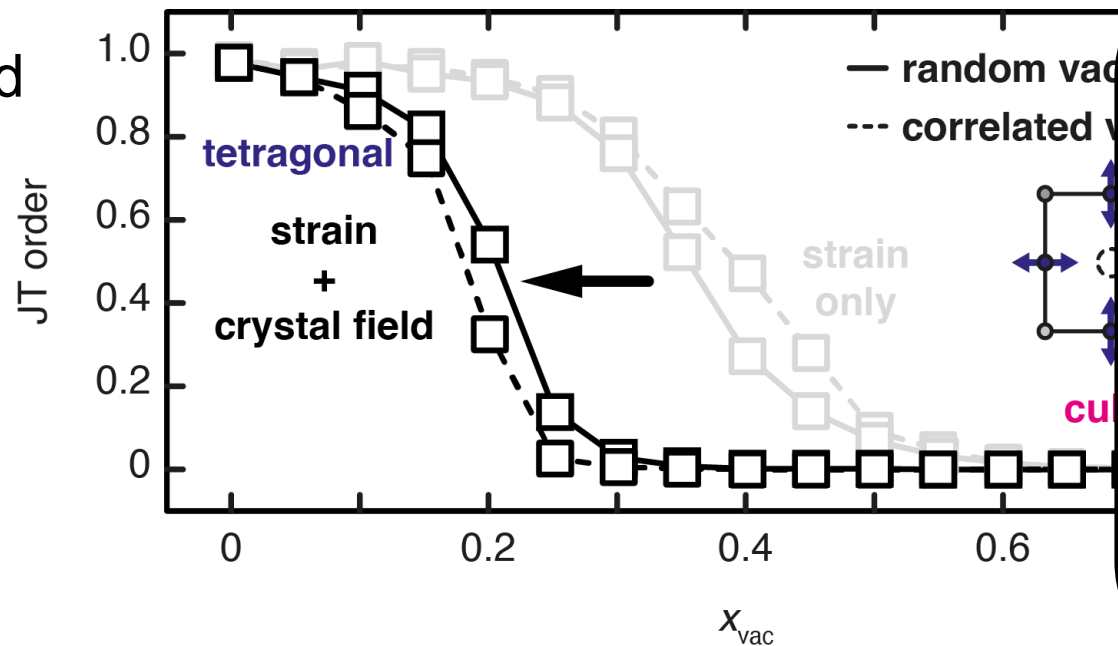
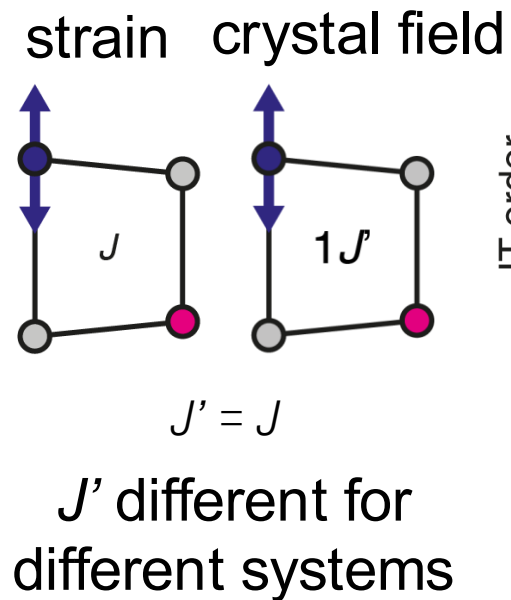
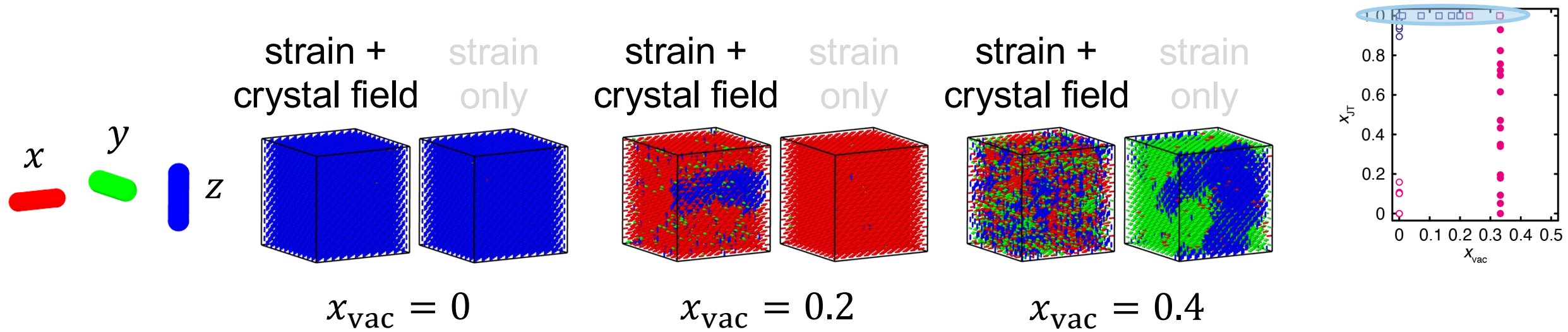
$\text{Cs}_{1-3x_{\text{vac}}}\text{Cu}[\text{Fe}(\text{CN})_6]_{1-x_{\text{vac}}}$: max JT, varying vacancies



critical (MC)
 $x_{\text{vac}} \approx 0.25$

critical
(experiment)
 $x_{\text{vac}} \approx 0.2$

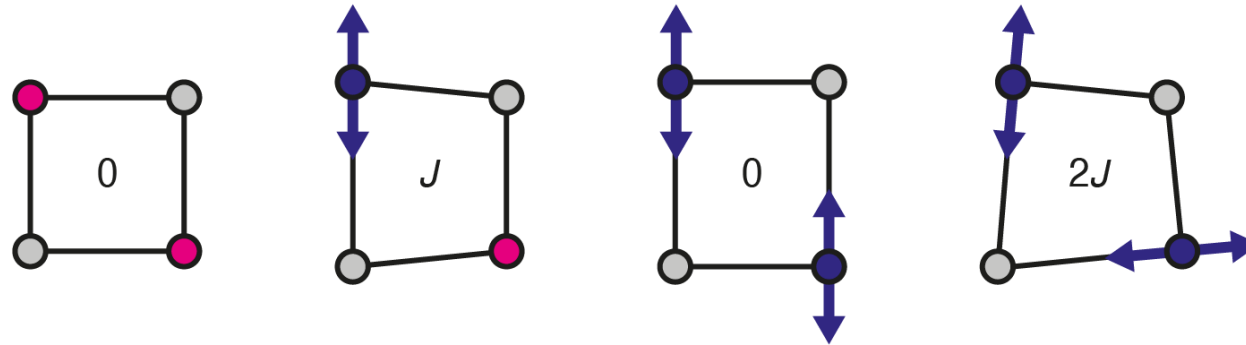
$\text{Cs}_{1-3x_{\text{vac}}}\text{Cu}[\text{Fe}(\text{CN})_6]_{1-x_{\text{vac}}}$: max JT, varying vacancies



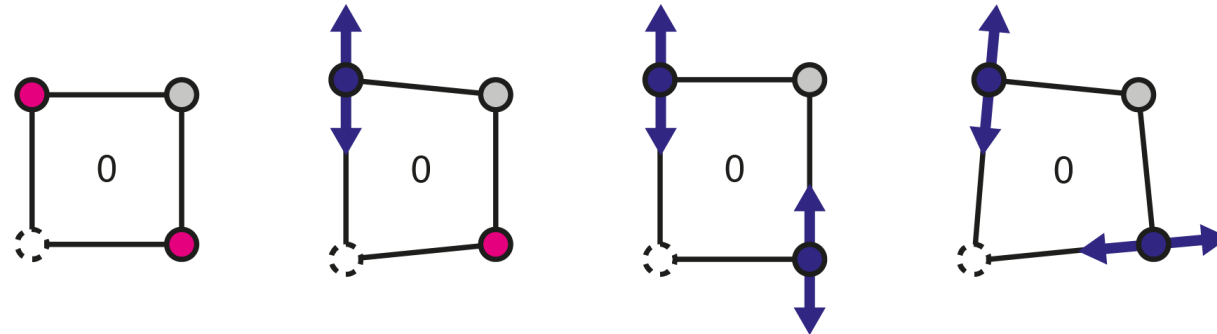
strain: JT coalignment
crystal-field: reorientation of JT axes towards vacancies

Rules

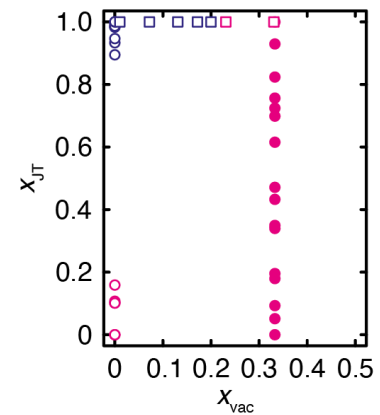
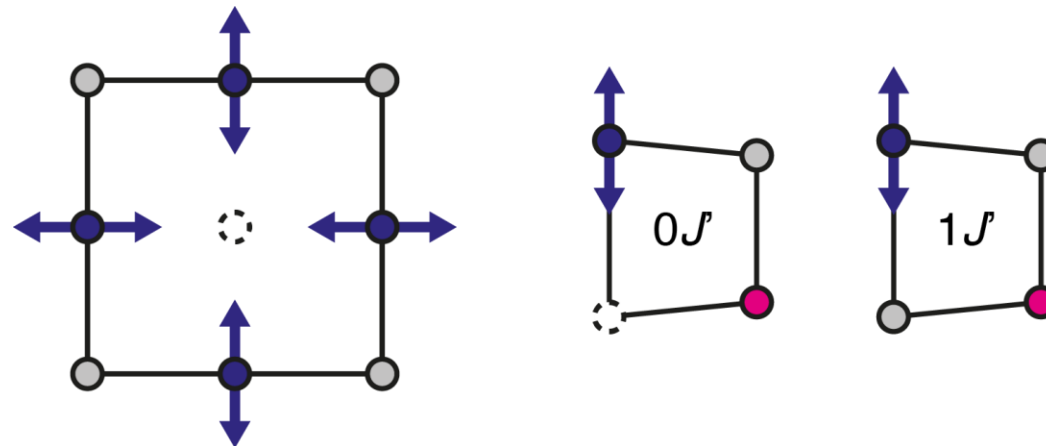
strain



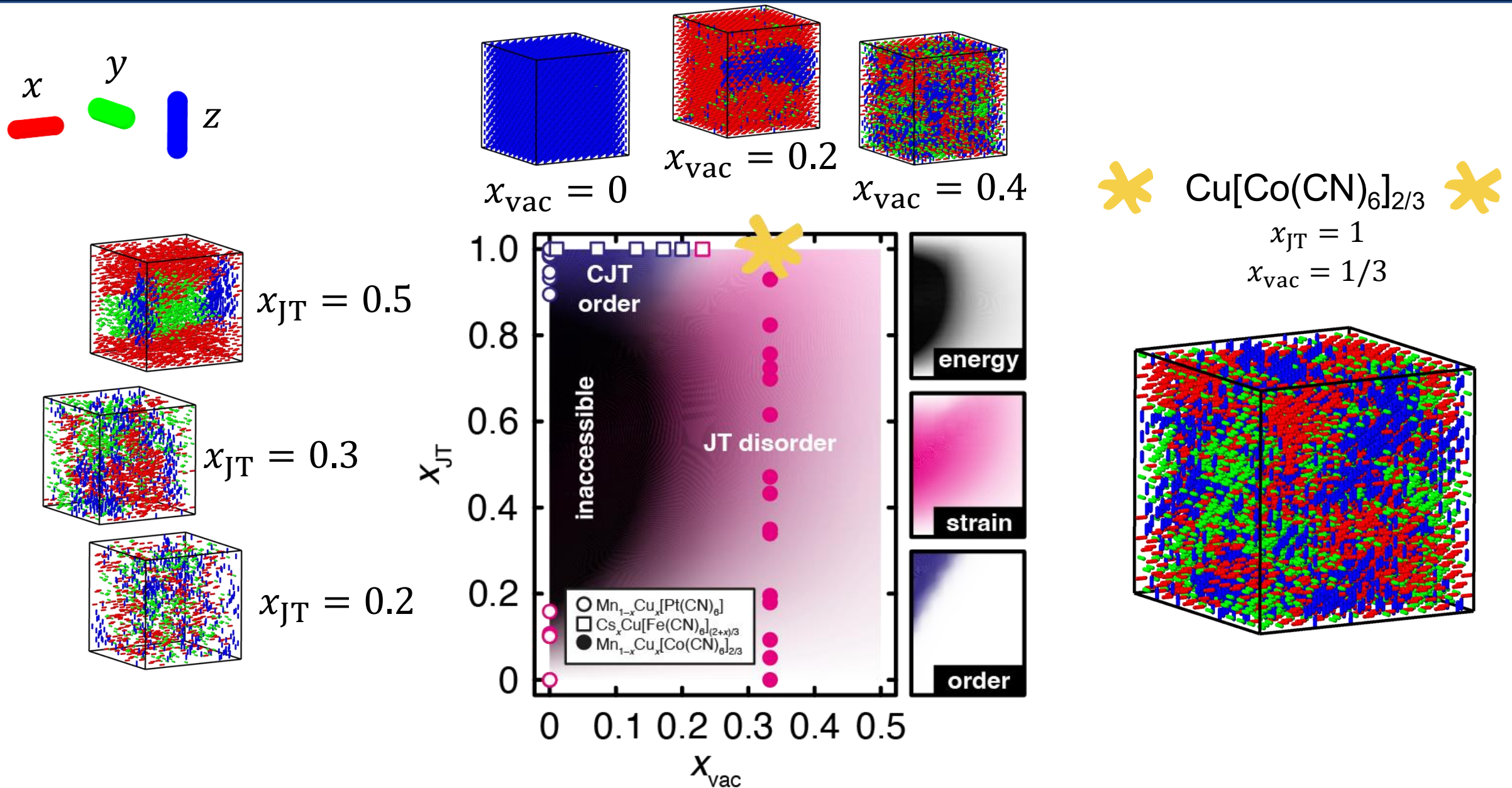
strain:
vacancies



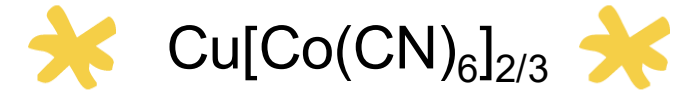
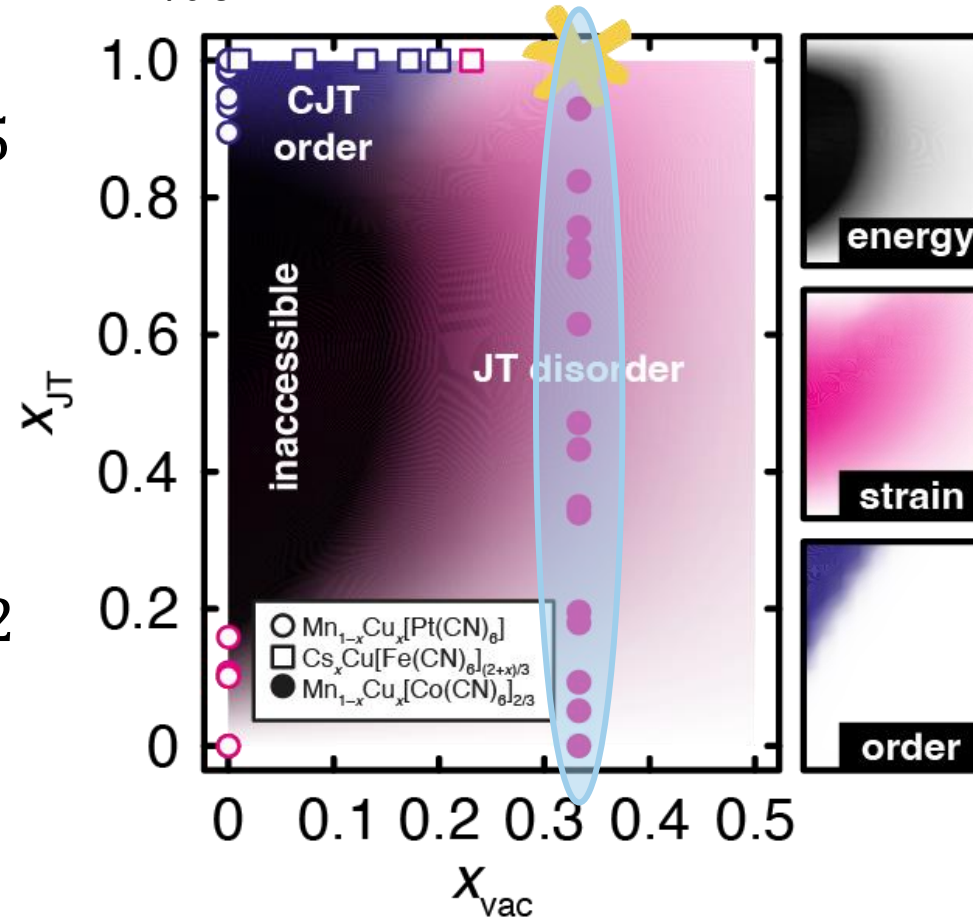
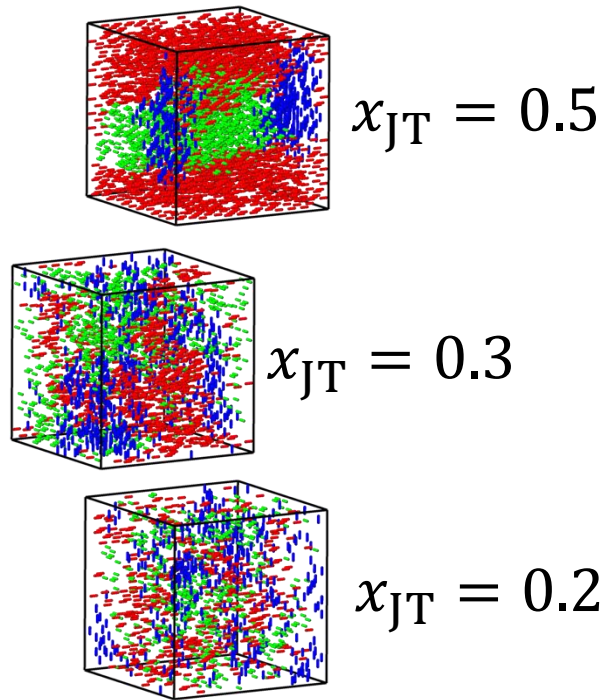
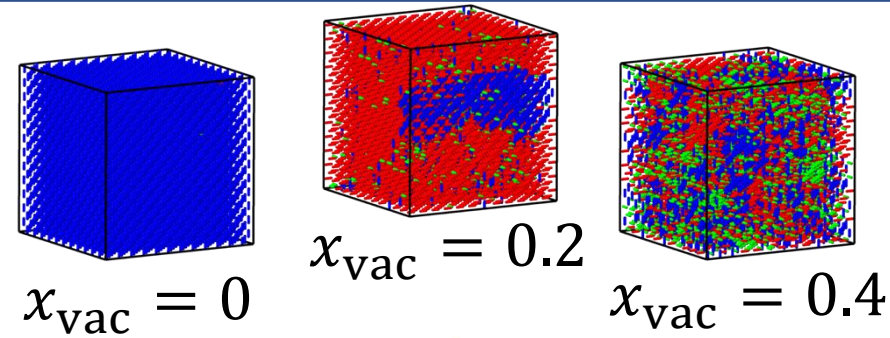
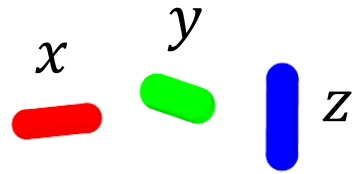
crystal-field



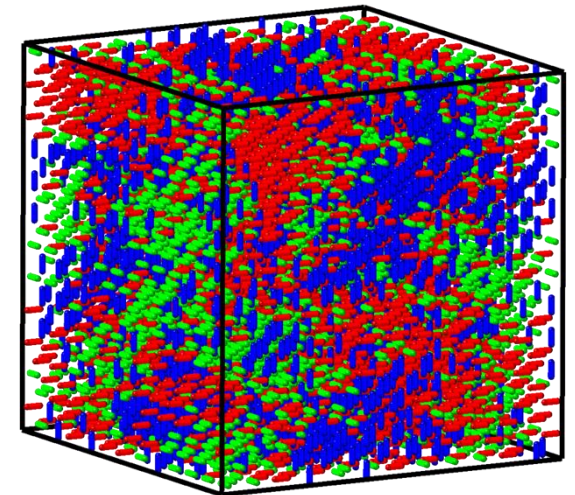
Phase map – interplay of JT/vacancy concentration



Phase map – interplay of JT/vacancy concentration



$x_{\text{JT}} = 1$
 $x_{\text{vac}} = 1/3$

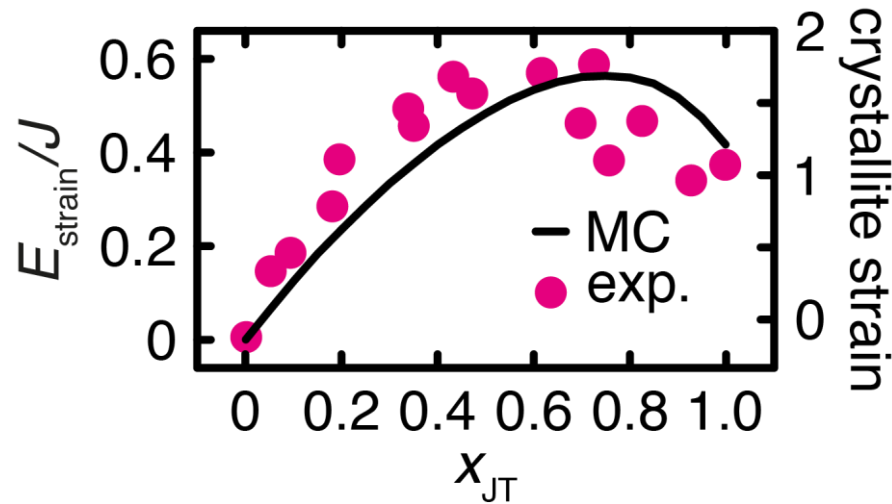
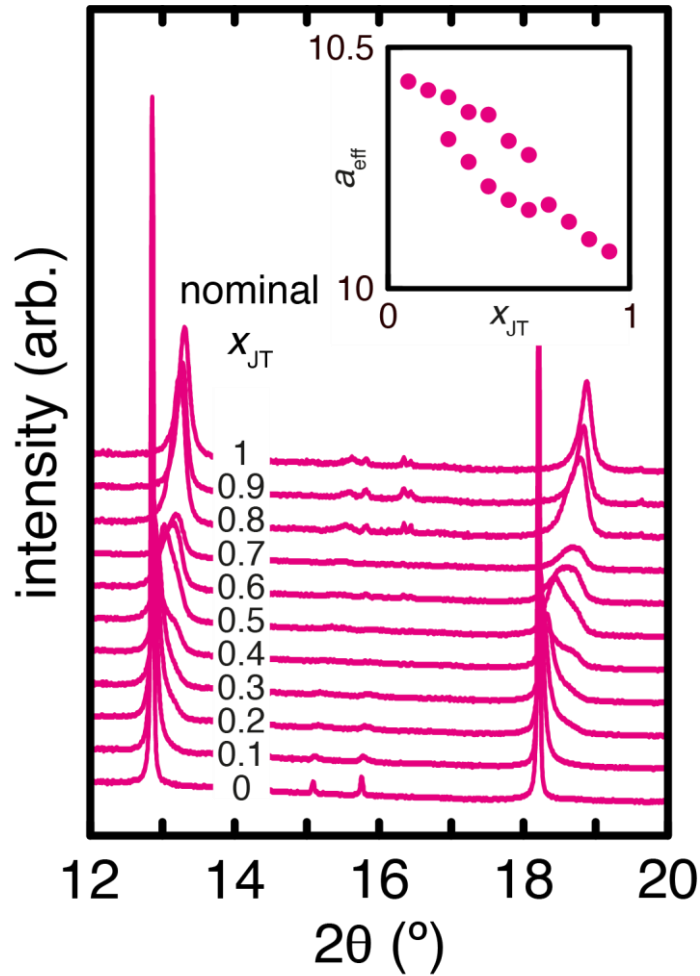
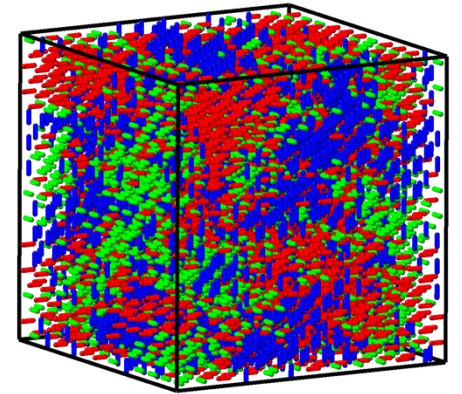


$(\text{Cu}_x\text{Mn}_{1-x})[\text{Co}(\text{CN})_6]_{2/3}$: $x_{\text{vac}} = 1/3$, vary JT

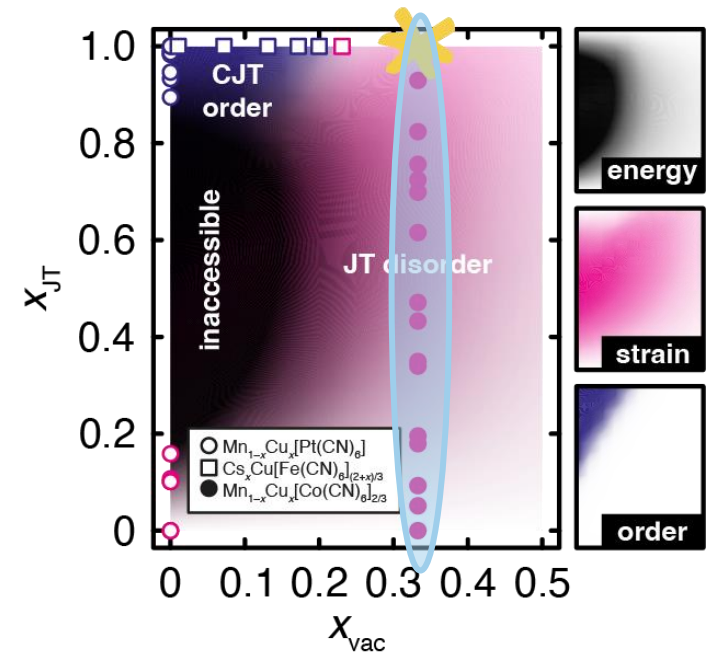
✱ $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$ ✱

$$x_{\text{JT}} = 1$$

$$x_{\text{vac}} = 1/3$$

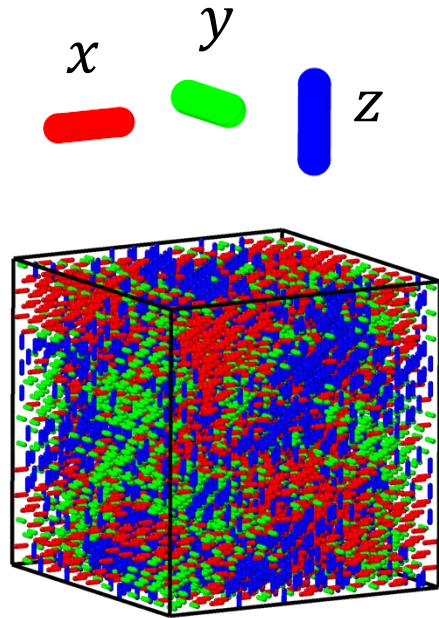


Isotropic crystal strain:
asymmetric dependence on x_{JT}
→ non-random JT
orientations/**local** JT order?

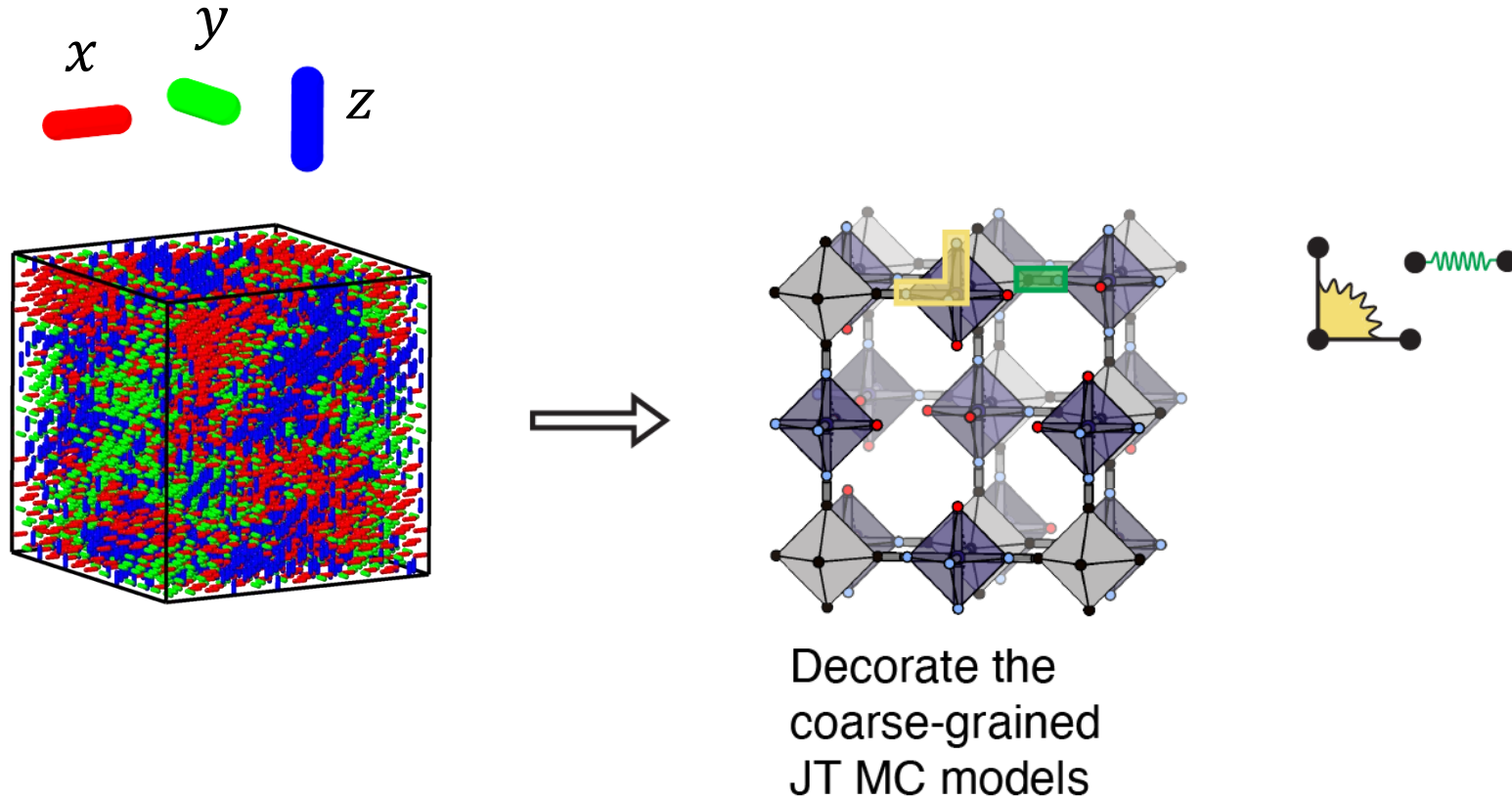


Solid-solutions, all **cubic**

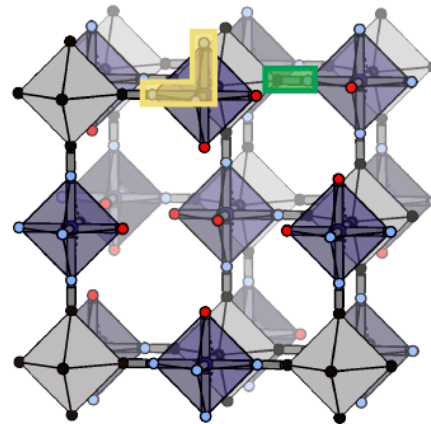
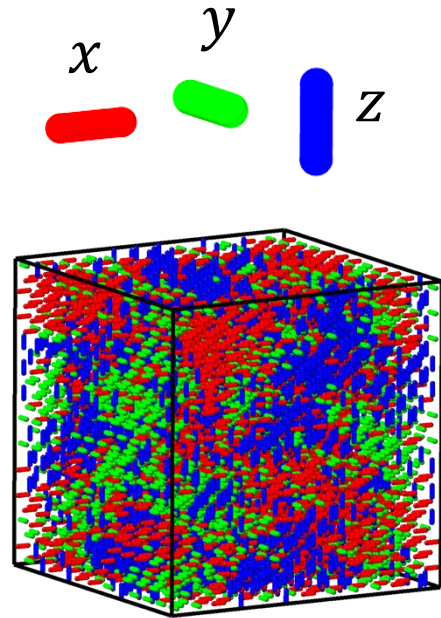
MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$

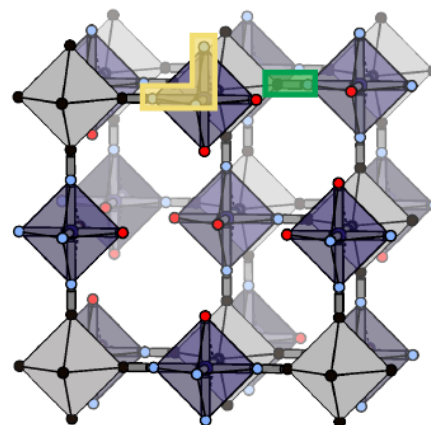
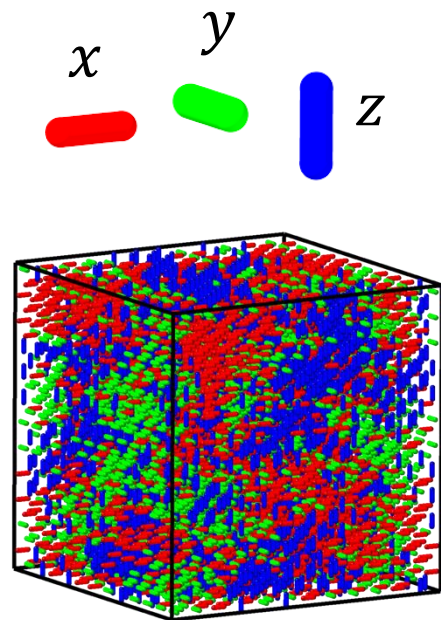


Decorate the
coarse-grained
JT MC models

Relax the configuration
using simple harmonic
bond and angle restraints

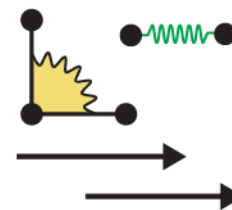


MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



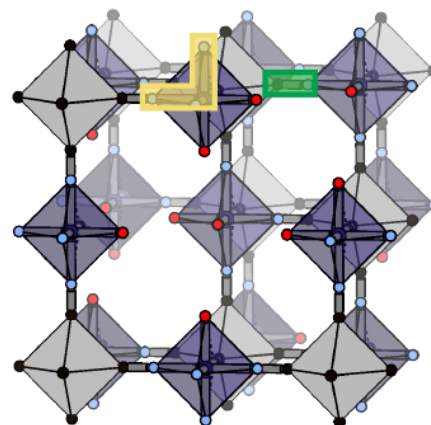
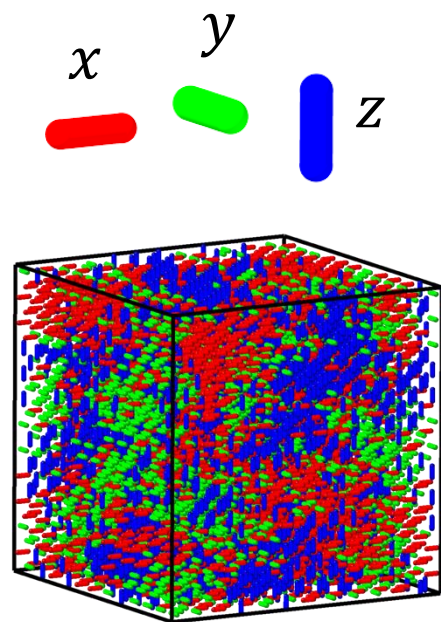
Decorate the
coarse-grained
JT MC models

Relax the configuration
using simple harmonic
bond and angle restraints



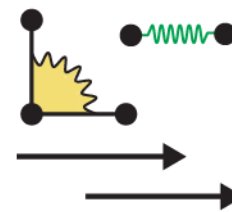
Refine parameters
(using MC-driven
big-box modelling
technique)

MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$

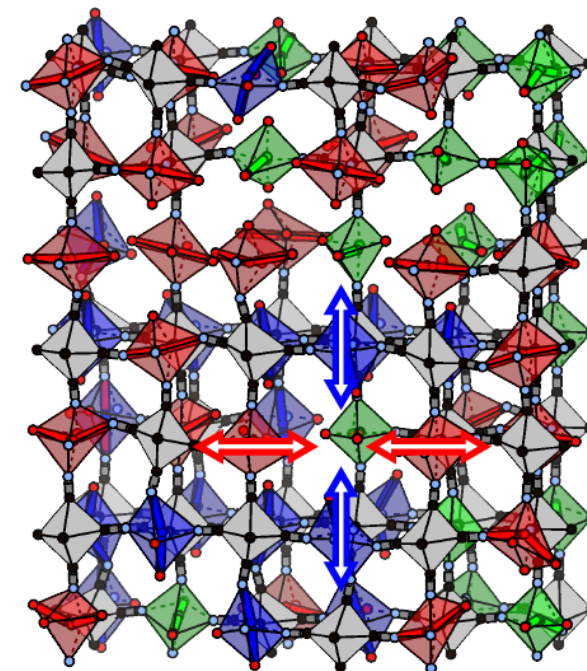


Decorate the
coarse-grained
JT MC models

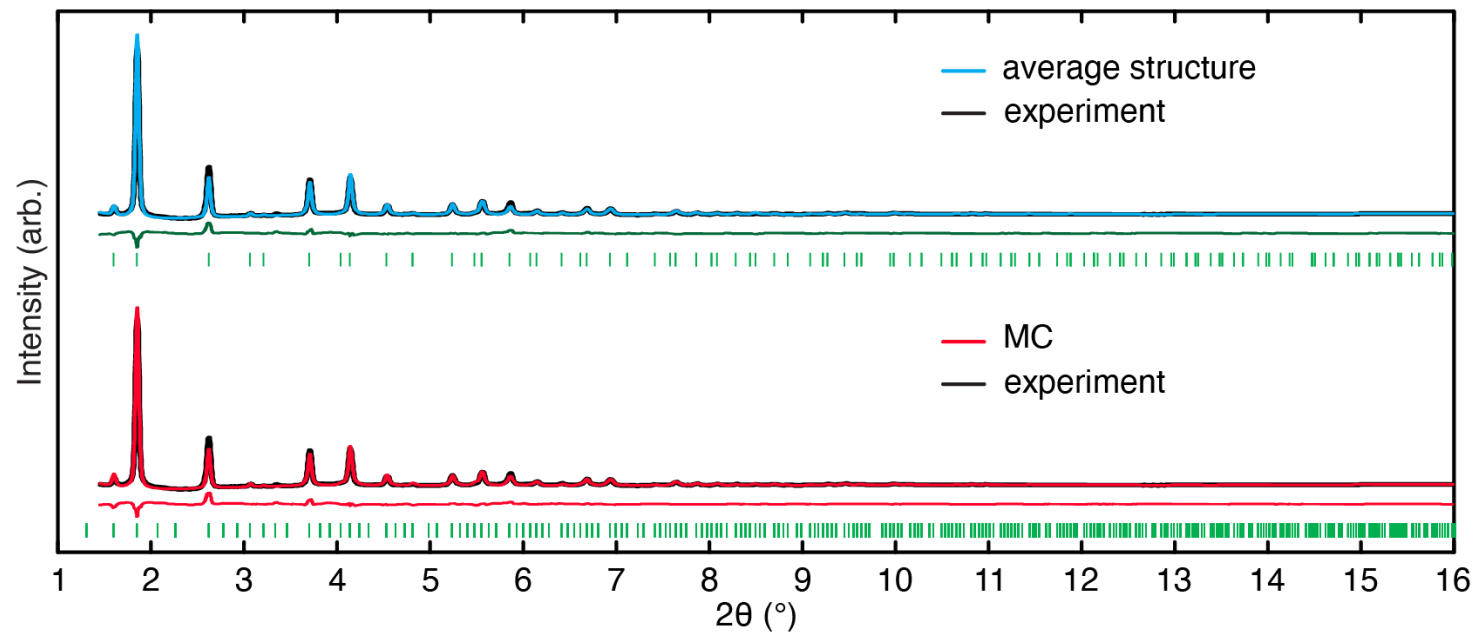
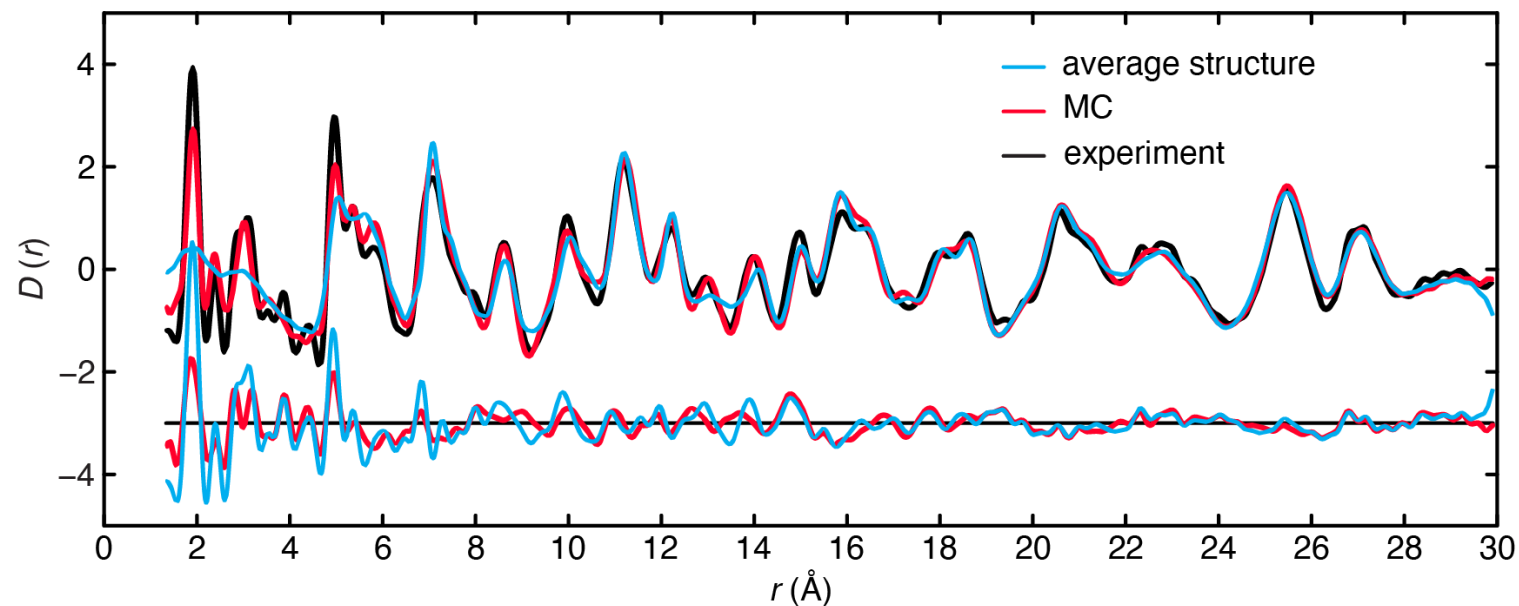
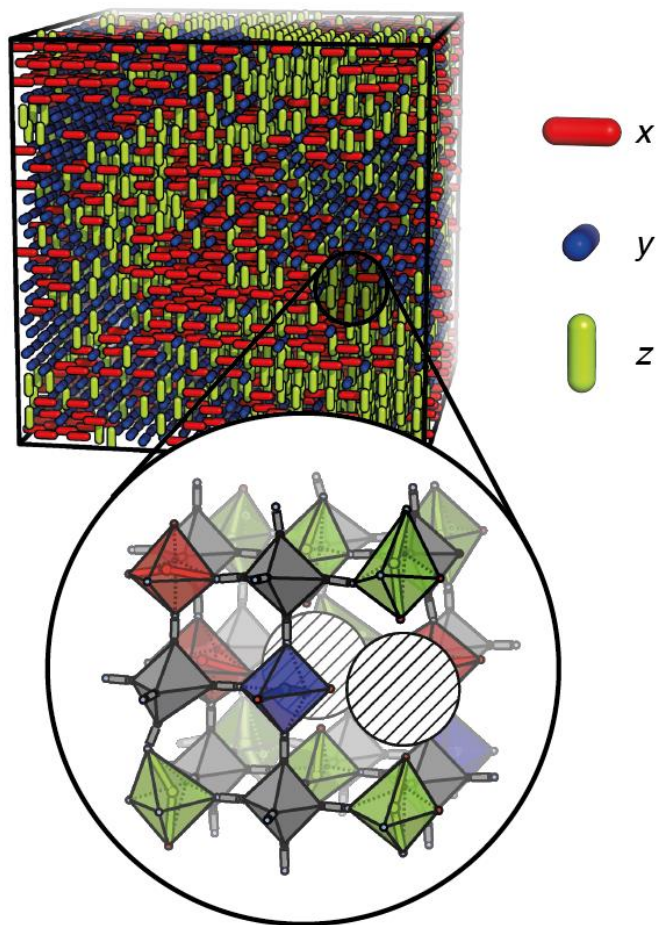
Relax the configuration
using simple harmonic
bond and angle restraints



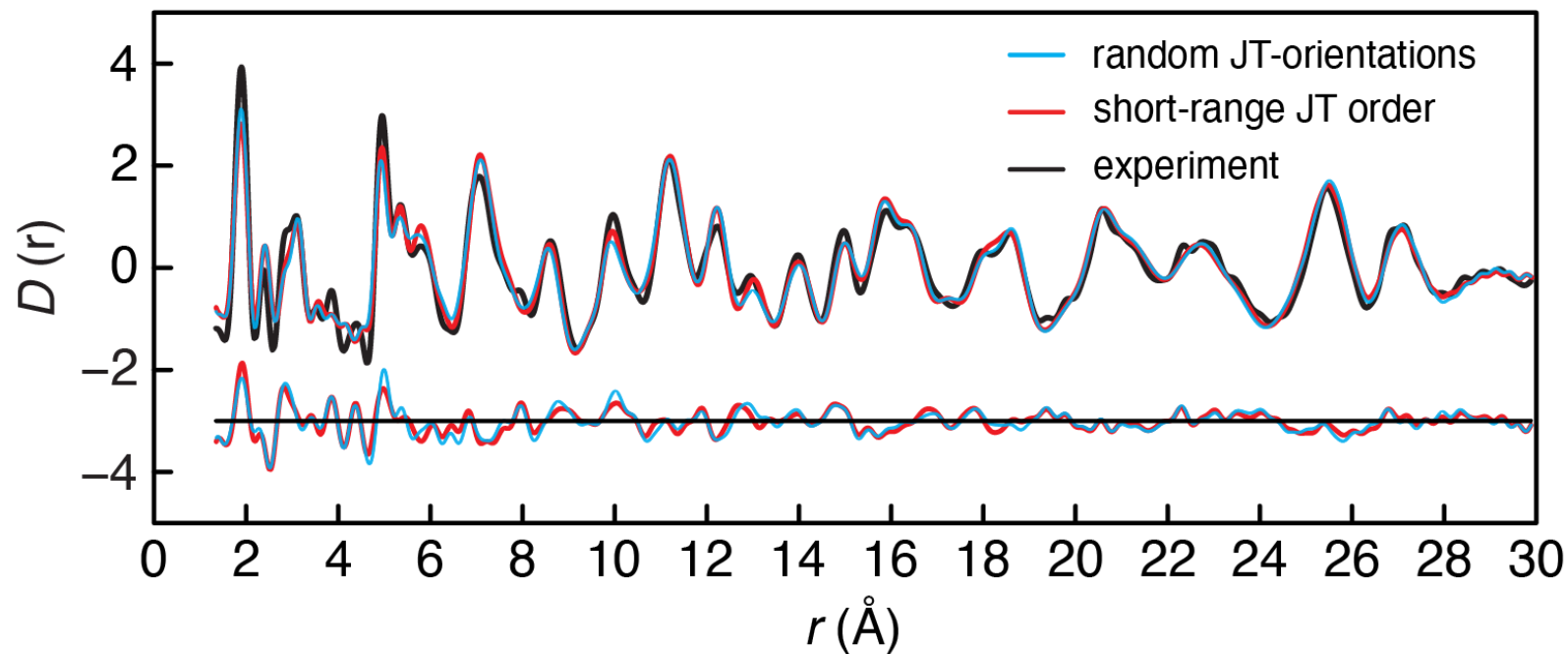
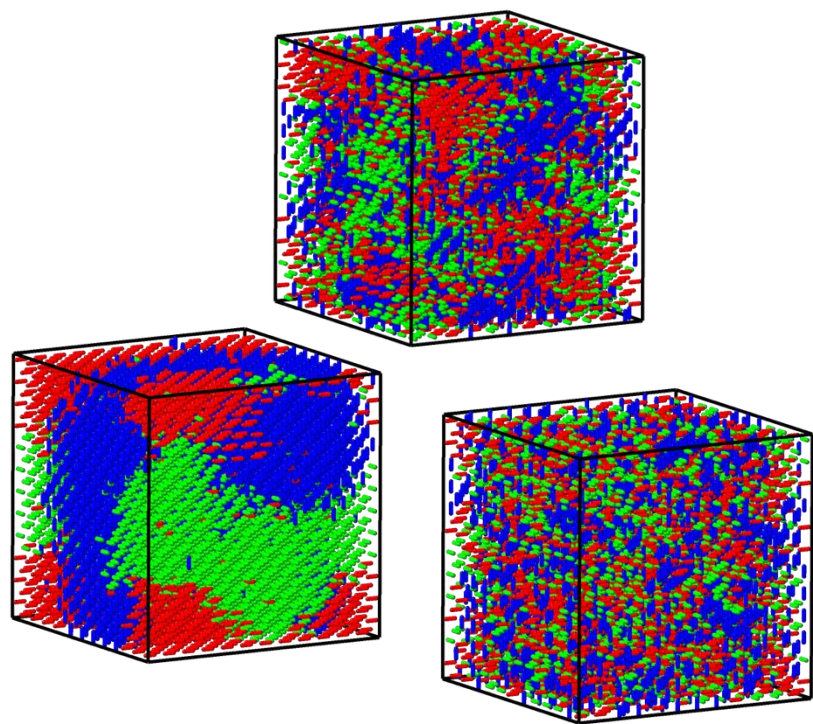
Refine parameters
(using MC-driven
big-box modelling
technique)



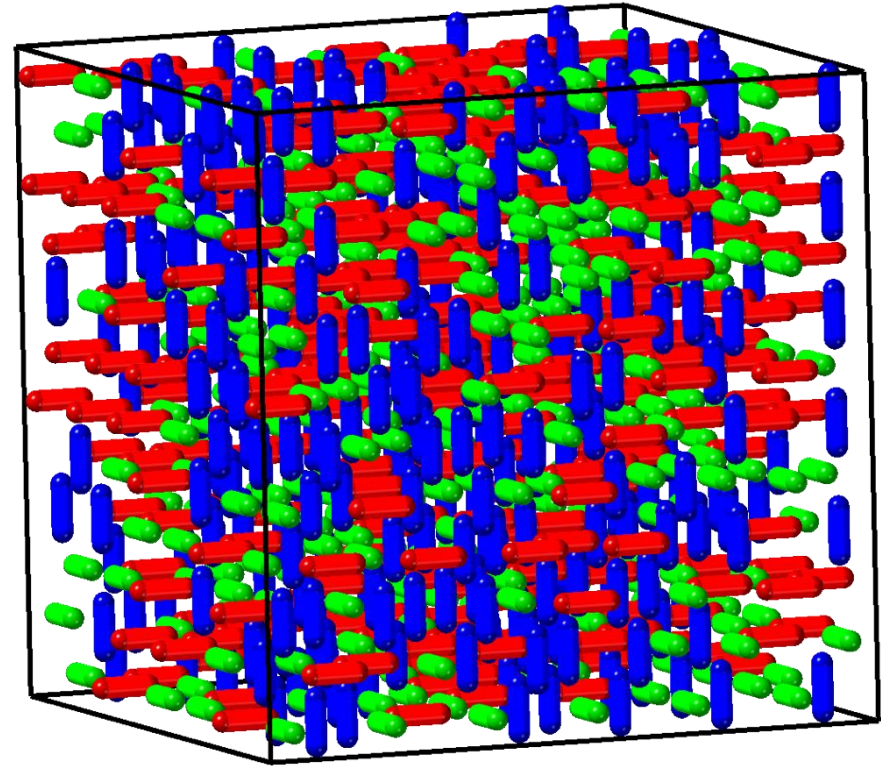
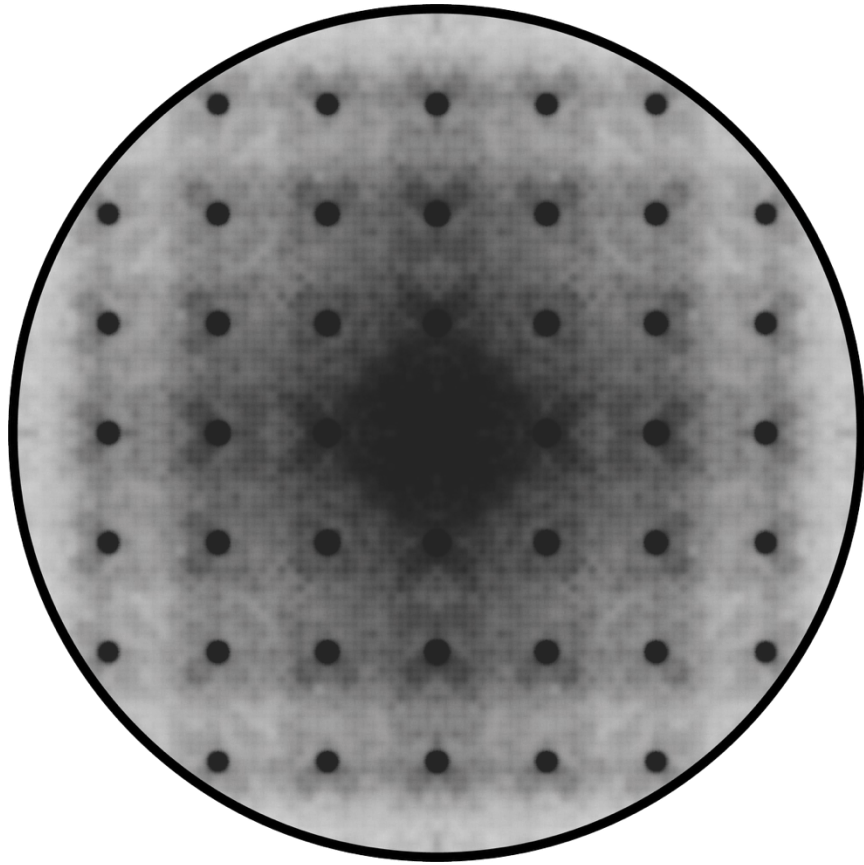
MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



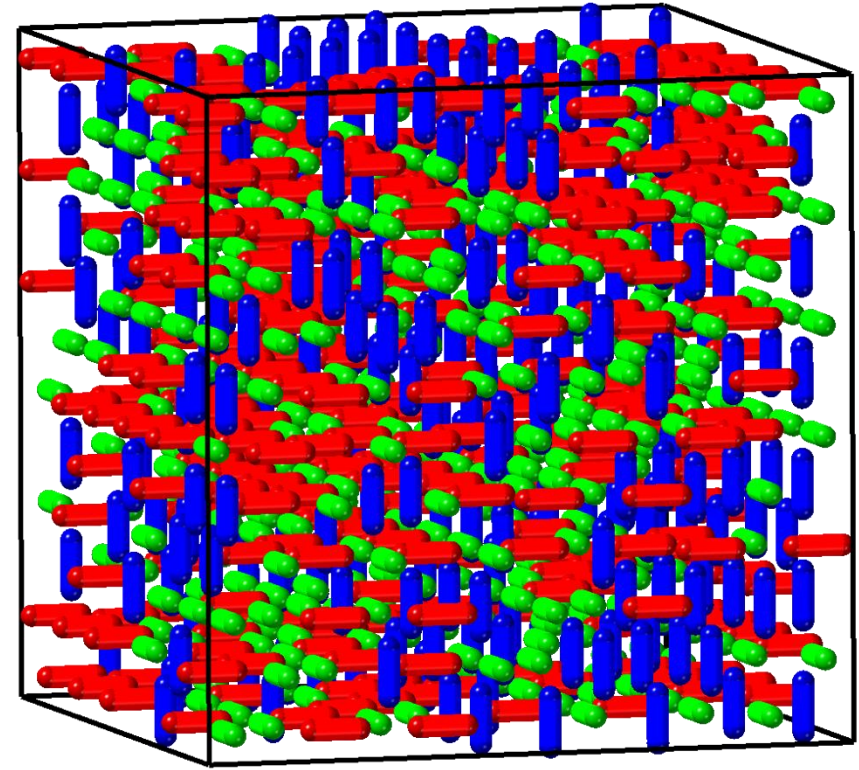
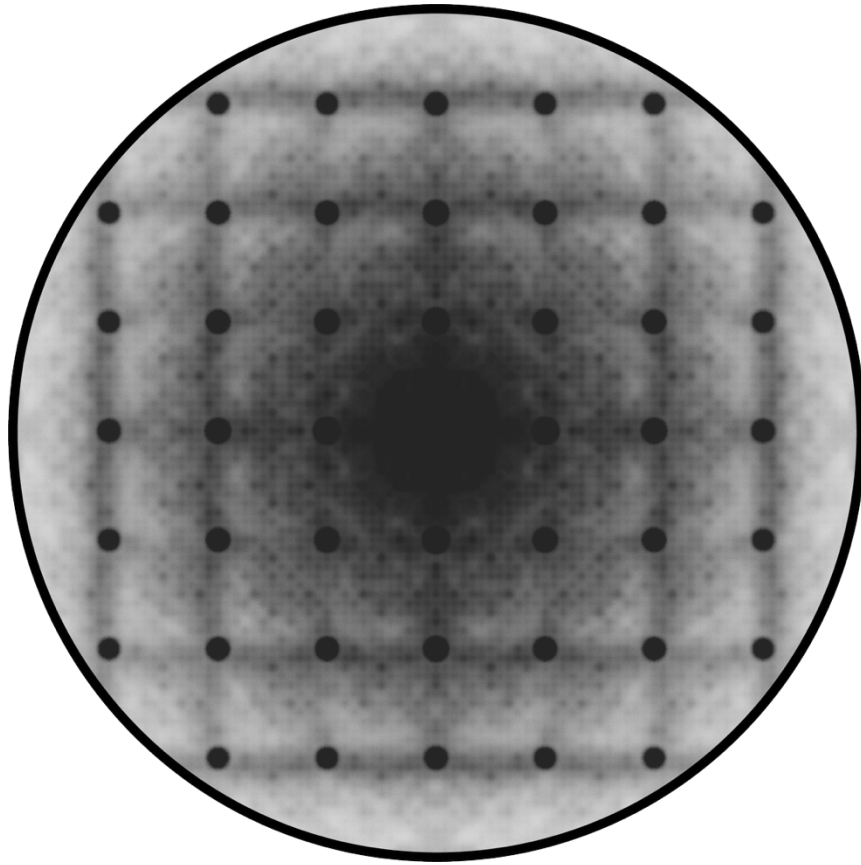
MC-driven big-box modelling – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



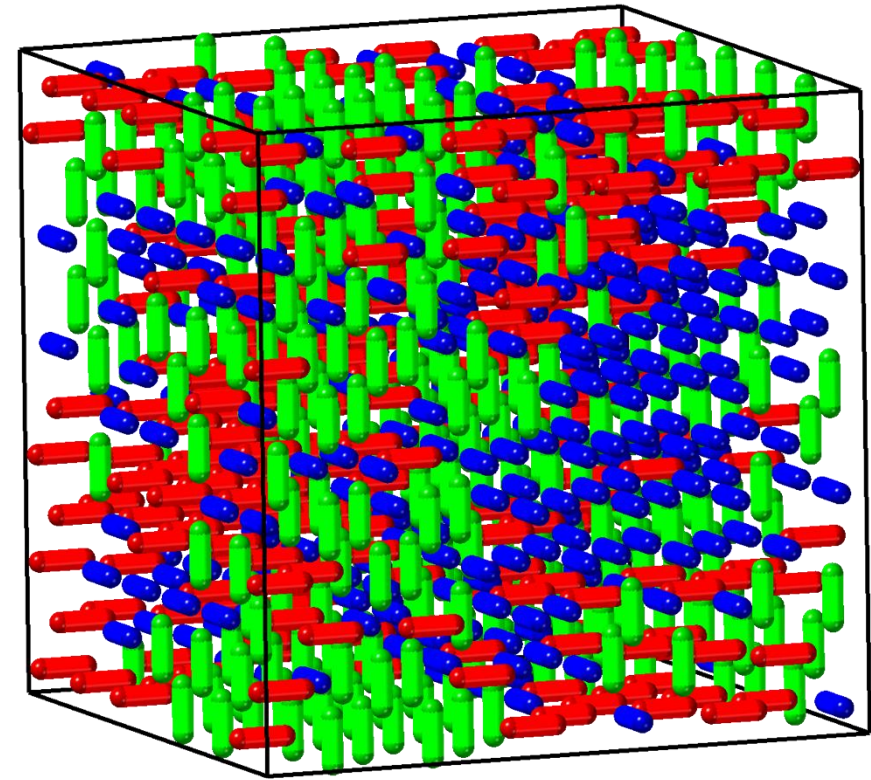
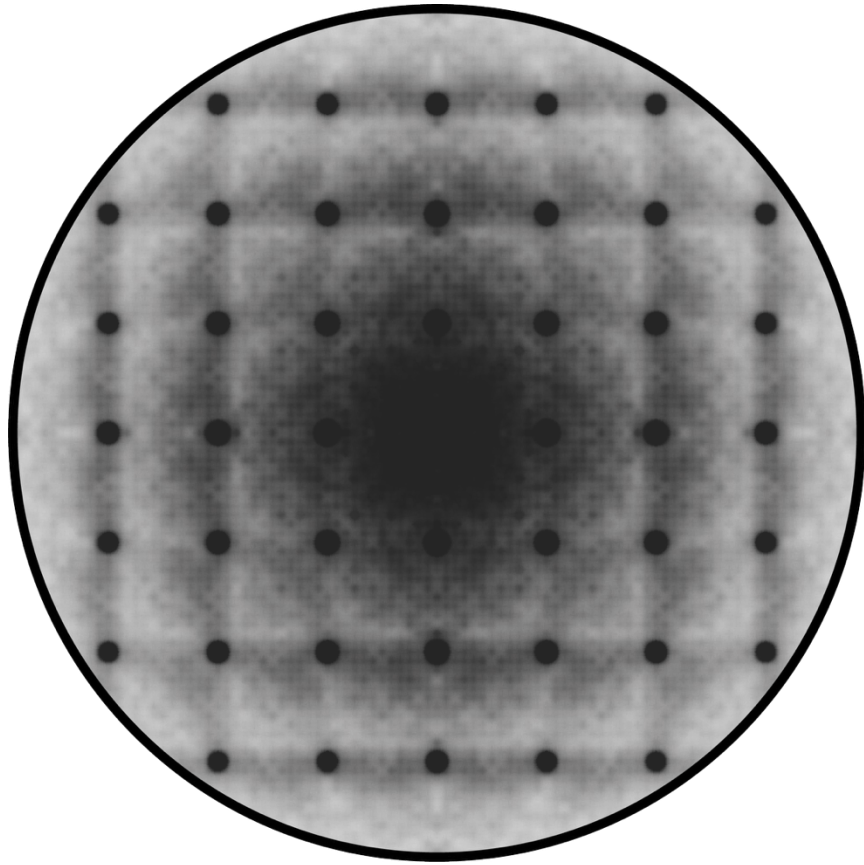
Single crystal pattern simulation – random vacancies – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



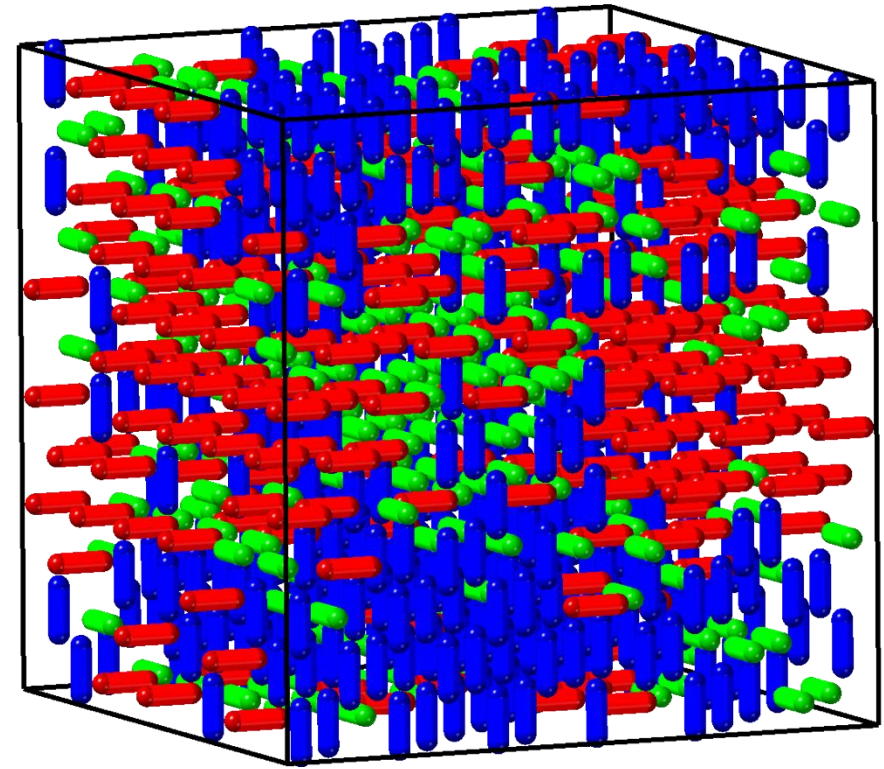
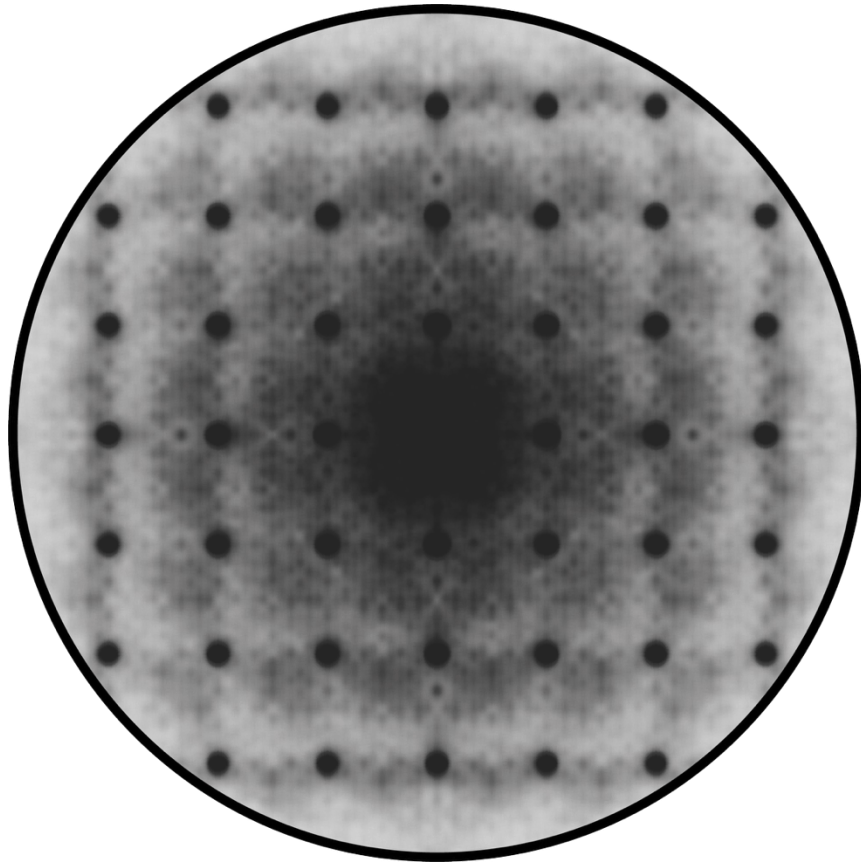
Single crystal pattern simulation – random vacancies – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



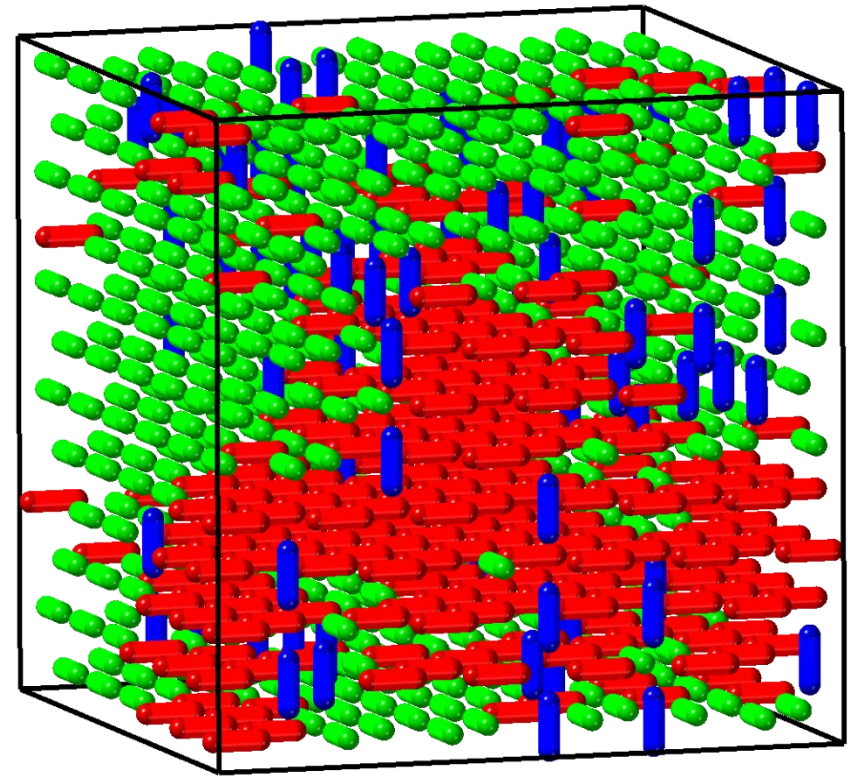
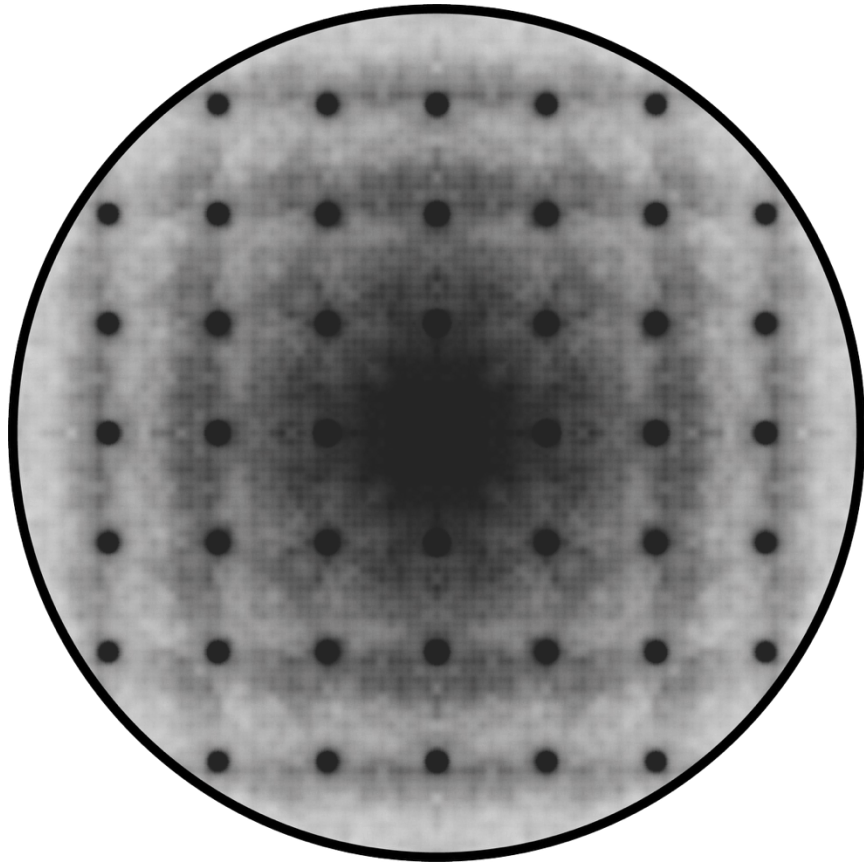
Single crystal pattern simulation – random vacancies – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



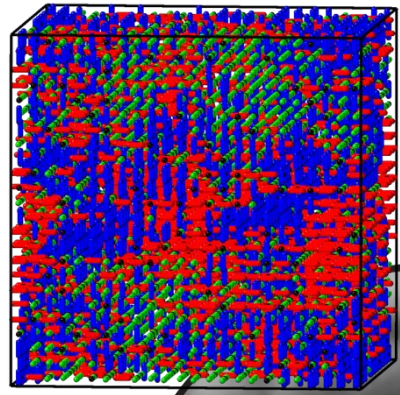
Single crystal pattern simulation – random vacancies – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



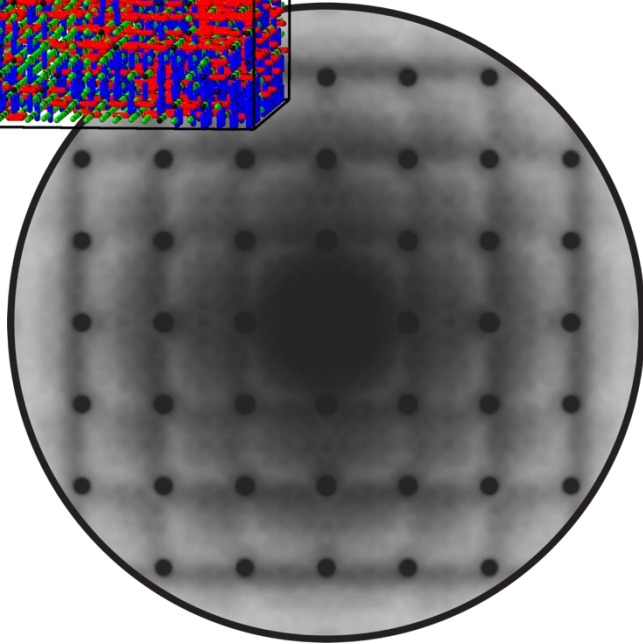
Single crystal pattern simulation – random vacancies – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



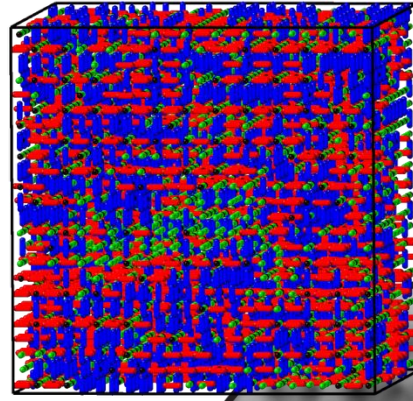
Single crystal – $\text{Cu}[\text{Co}(\text{CN})_6]_{2/3}$



Simulated
 $J' = 1$

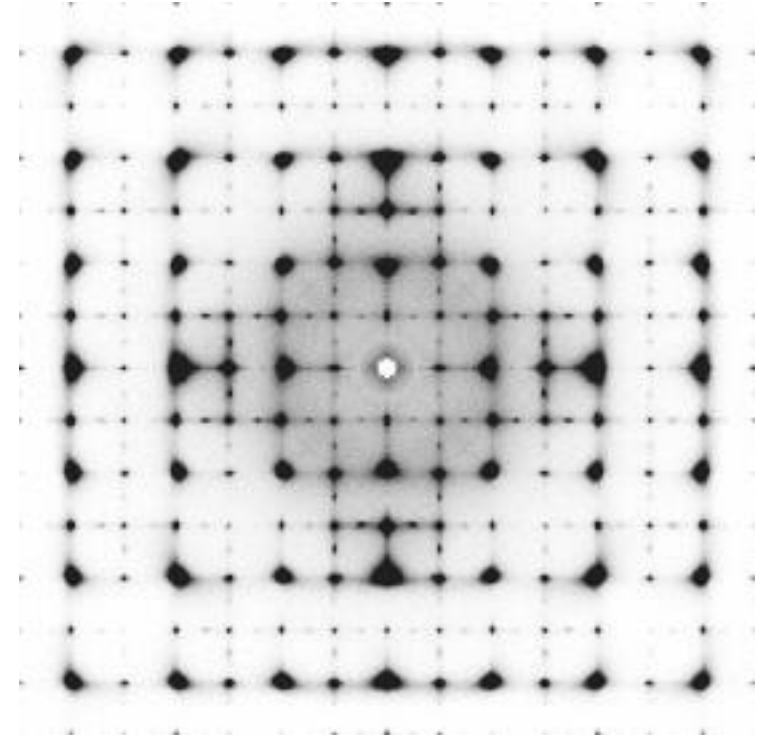


Random vacancies



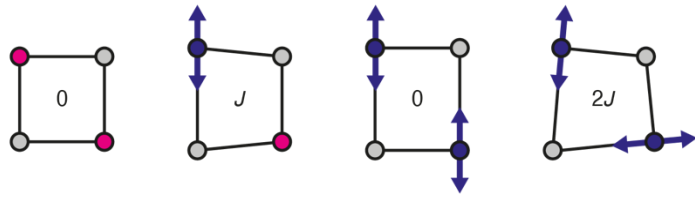
Correlated vacancies

Experiment

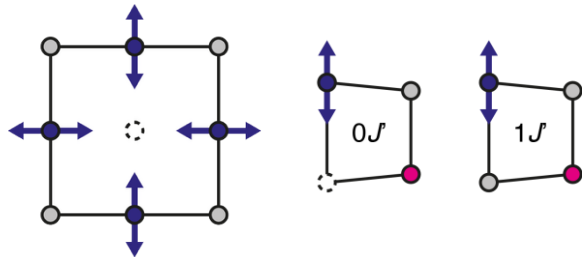


Simonov *et al*, *Nature* **2020**,
578, 256

Conclusions

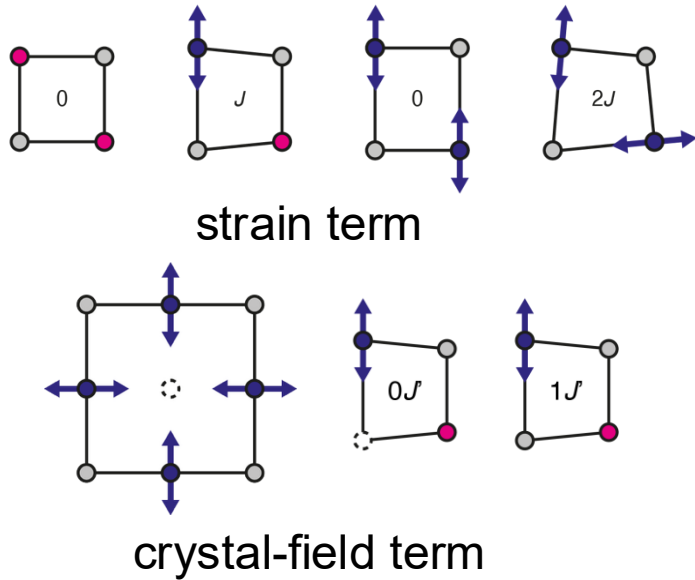


strain term



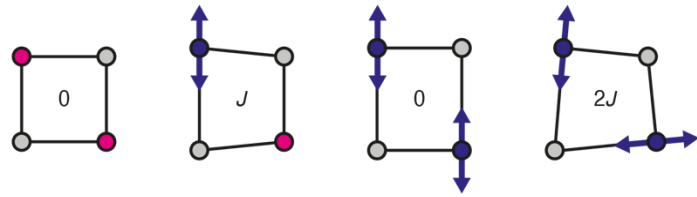
crystal-field term

Conclusions

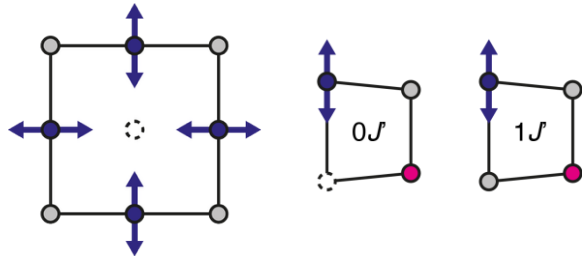


- A **simple model** governing cooperative JT order based on the competition between **strain** and **crystal-field** stabilisation.

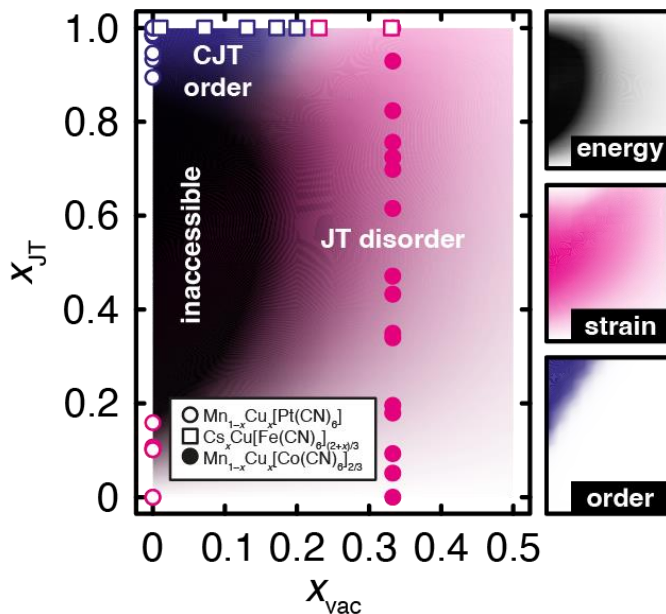
Conclusions



strain term



crystal-field term



- A **simple model** governing cooperative JT order based on the competition between **strain** and **crystal-field** stabilisation.
- Can **account** for the extent of cooperative JT order, crystallite strain, and stability **measured experimentally**.
- Generic **phase map** – gives an indication of how PBA **compositions** might be **tuned** to control the emergence of long-range cooperative JT order.

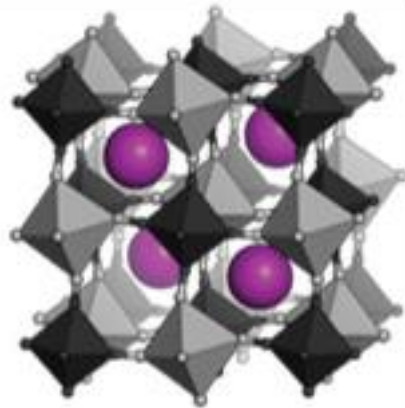
Conclusions

PBAs contain a complex interplay of competing effects



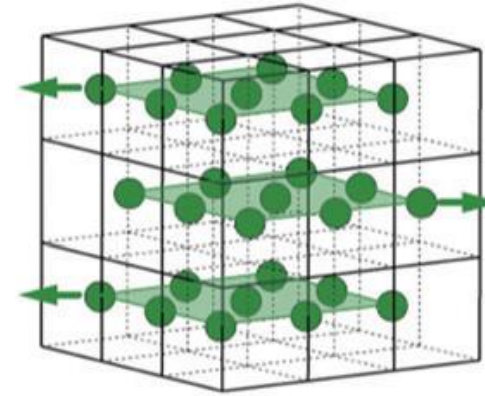
Correlated vacancies

Simonov *et al*,
Nature **2020**,
578, 256



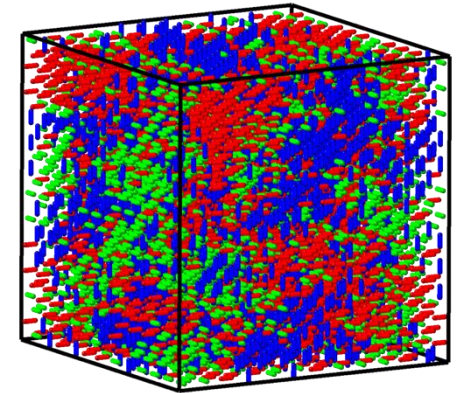
Octahedral tilts

Boström & Brant,
J. Mater. Chem. C.
2022, 10, 13690



A-site 'slides'

Cattermull *et al*,
JACS **2023**, 145,
24249



Cooperative JT

This work
arXiv:2408.13169
2024

Cattermull, Pasta, Goodwin, *Mater. Horiz.*, **2021**, 8, 3178
Cattermull, Pasta, Goodwin, *J. Am. Chem. Soc.* **2023**, 145, 24471



Science and
Technology
Facilities Council

Acknowledgements

DEPARTMENT OF
CHEMISTRY



Helena Barker
(Oxford)



Quentin Guérout
(Oxford)



John Cattermull
(Oxford)



Hanna Boström
(Oxford/Stockholm)



Rebecca Witte
(Oxford)



Liam Nagle-Cocco
(Cambridge)



John Evans
(Durham)



Nikolaj Roth
(Oxford/Aarhus)



David Keen
(ISIS)



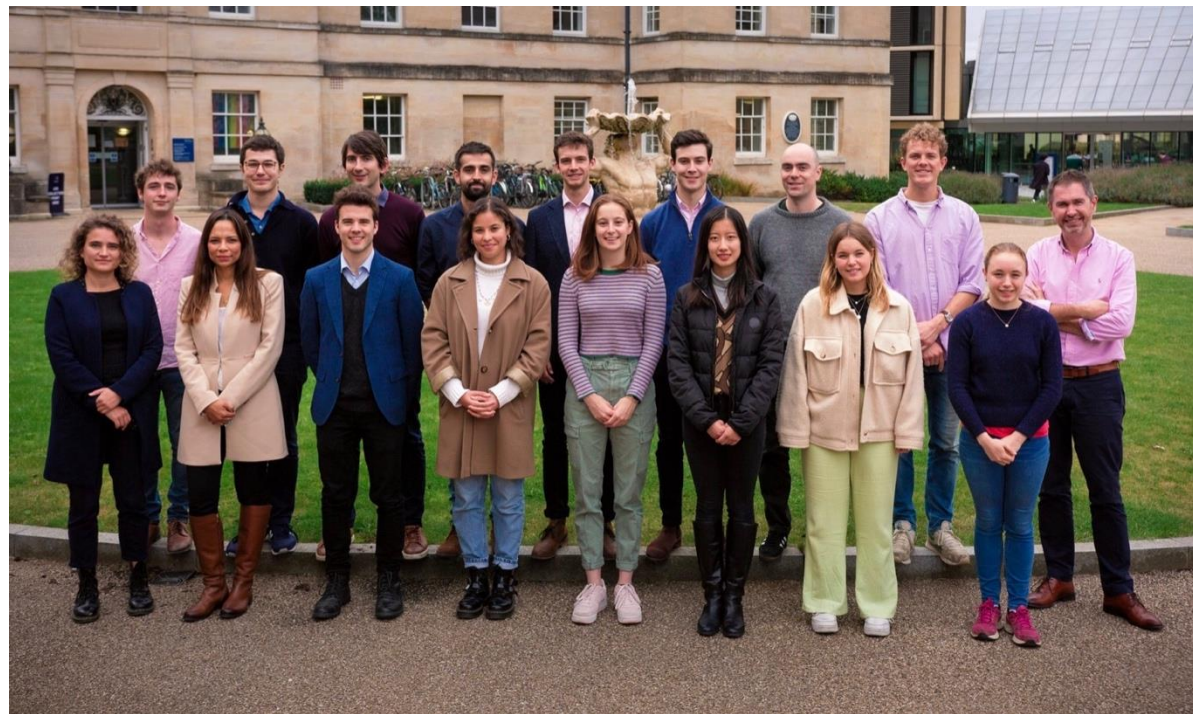
Andrew Goodwin
(Oxford)



Science and
Technology
Facilities Council

Acknowledgements

DEPARTMENT OF
CHEMISTRY



2022



2025

Goodwin Group