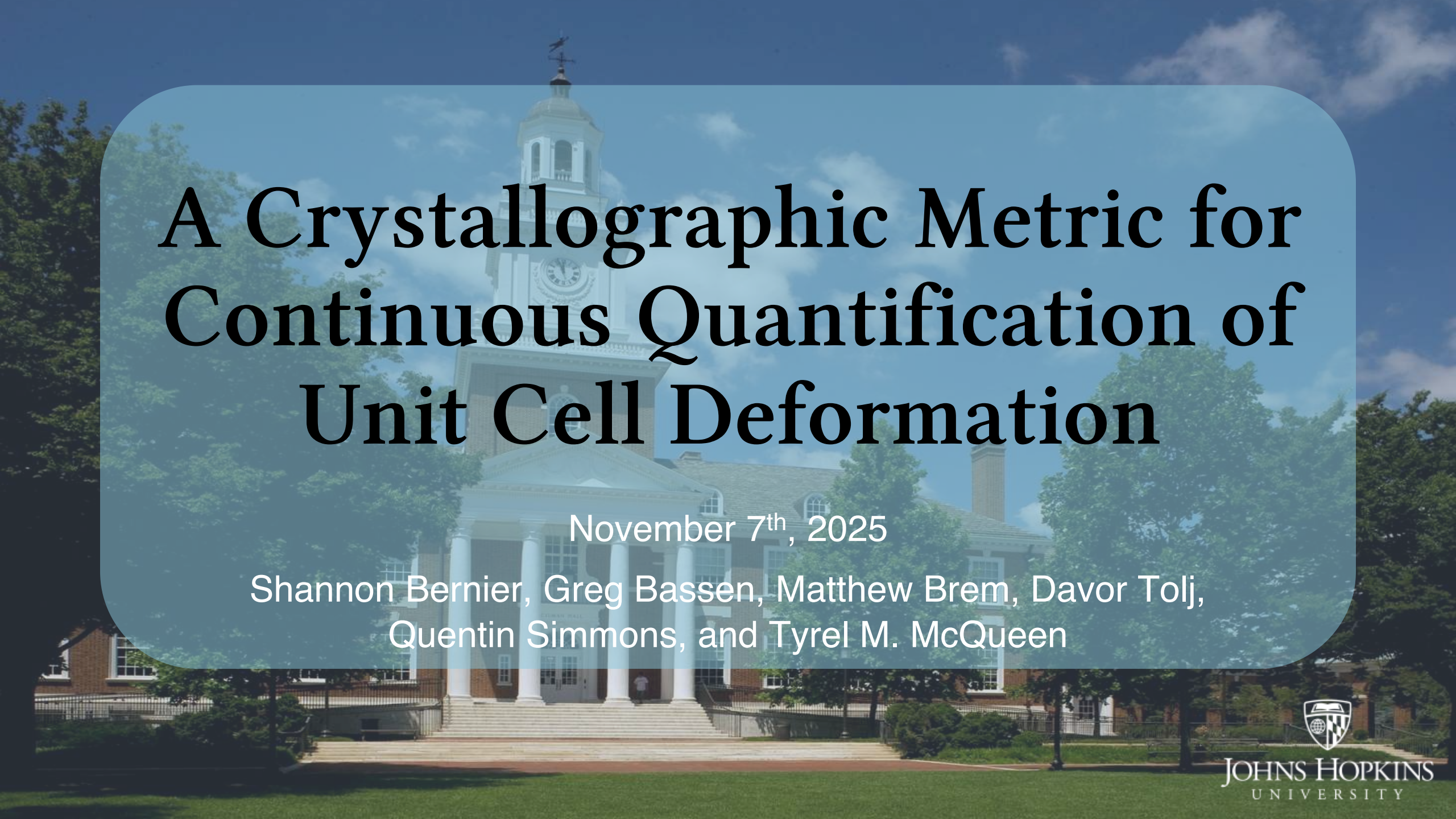

A Crystallographic Metric for Continuous Quantification of Unit Cell Deformation

November 7th, 2025

Shannon Bernier, Greg Bassen, Matthew Brem, Davor Tolj, Quentin Simmons, and Tyrel M. McQueen

JOHNS HOPKINS UNIVERSITY

Funding & collaborators

Principal Investigator


Tyrel M. McQueen


Shannon Bernier


Greg Bassen


Davor Tolj


Quentin Simmons


Matthew Brem

Geometry & proofs

Crystallography & applications

Materials synthesis

U.S. National Science Foundation

U.S. DEPARTMENT of ENERGY

C²QA

PARADIM
AN NSF MATERIALS INNOVATION PLATFORM

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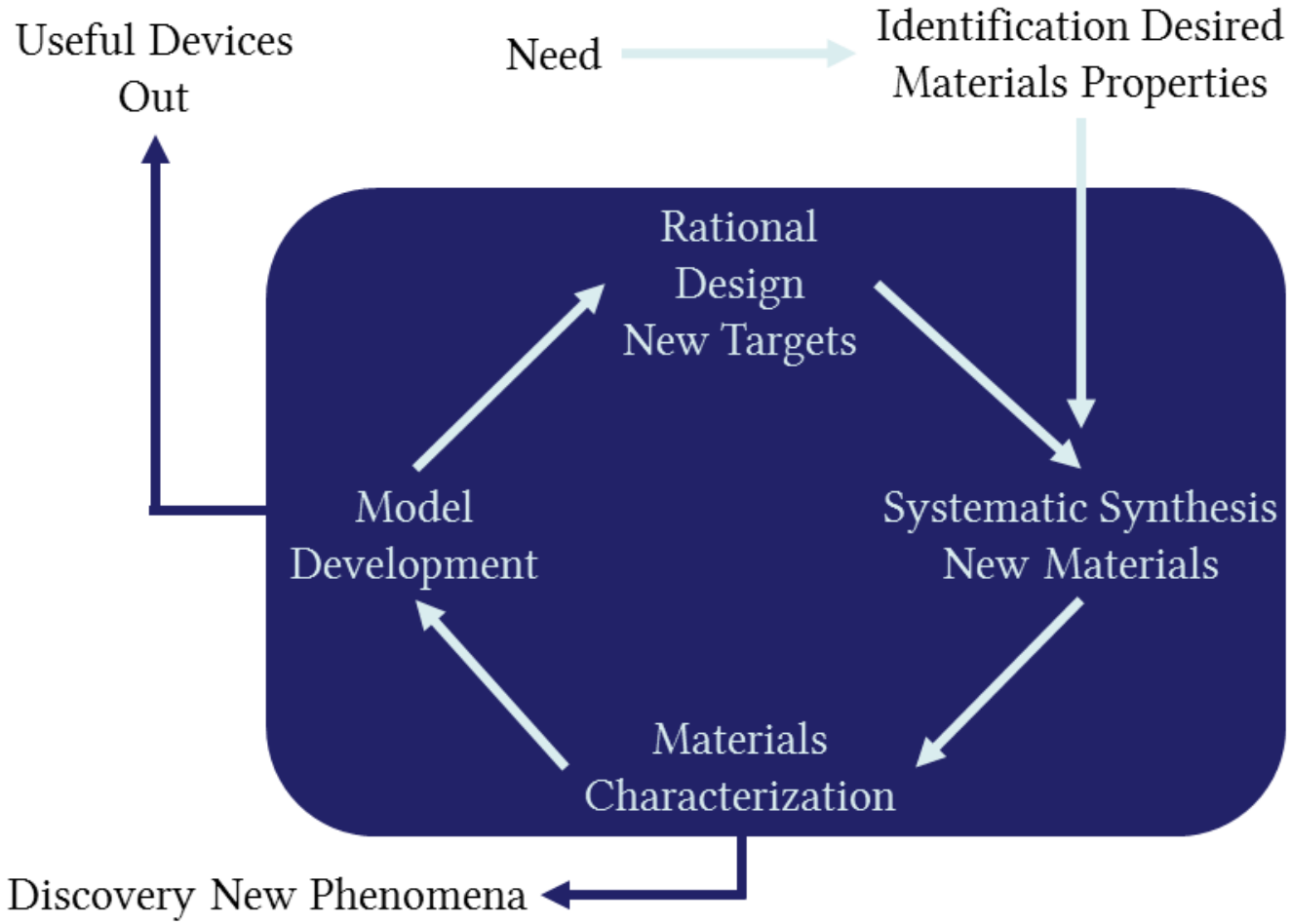
Materials lifecycle



McQueen Lab

Journal of the American Ceramic Society

ORIGINAL ARTICLE

$Bi_{0.5}K_{0.5}TiO_3$–$CaTiO_3$ ceramics: Appearance of the pseudocubic structure and ferroelectric-relaxor transition characters

Yongxing Wei, Ning Zhang, Changqing Jin, Weitong Zhu, Yiming Zeng, Gang Xu, Ling Gao, Zengyun Jian

Materials Research Bulletin

Volume 185, May 2025, 113318

cal models for predicting cubic/
ocubic lattice parameters of
perovskites

Home › MRS Online Proceedings Library › Article

Epitaxial Growth and Structure of Cubic and Pseudocubic Perovskite Films on Perovskite Substrates

Published: 15 February 2011

Volume 401, pages 109–114, (1995) Cite this article

Orbital Correlations in the Pseudocubic O and Rhombohedral R Phases of $LaMnO_3$

angyun [redacted][1], T[redacted]en[2], J[redacted], and S. J. L. Billinge[1]

Show more

Phys. Rev. Lett. **94**, 177203 – **Published 5 May, 2005**

pseudocubic

Designing pseudocubic perovskites with enhanced nanoscale polarization FREE

I. Levin; W. J. Laws; D. Wang; I. M. Reaney

Check for updates

+ Author & Article Information

Appl. Phys. Lett. 111, 212902 (2017)

Evidence of pseudocubic structure in sol-gel derived $Pb_{1-x}Ca_xTiO_3$ $(x = 0.35–0.48)$ ceramic by dielectric and Raman spectroscopy

Arun Singh; K. Sreenivas; R. S. Katiyar; Vinay Gupta

Check for updates

+ Author & Article Information

J. Appl. Phys. 102, 074110 (2007)

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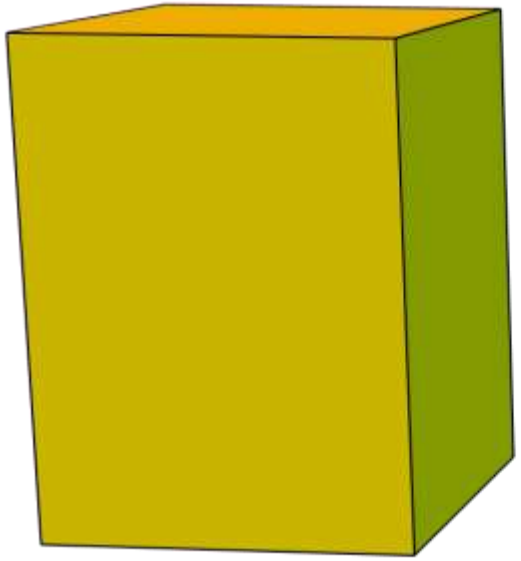
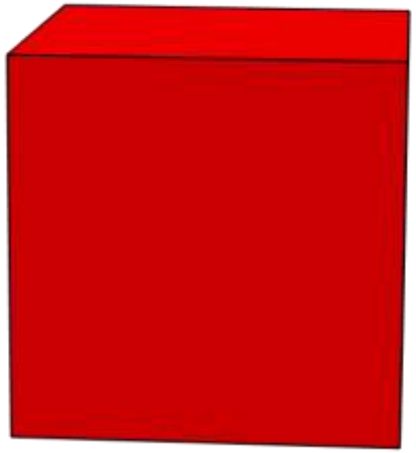
Which is more cubic?

✗ Equal lengths
✓ Equal angles



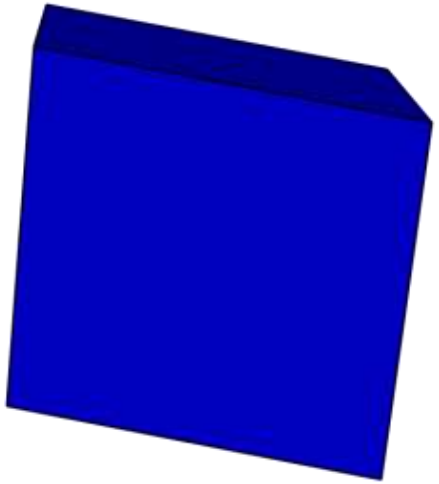
Rectangular prism

✓ Equal lengths
✓ Equal angles



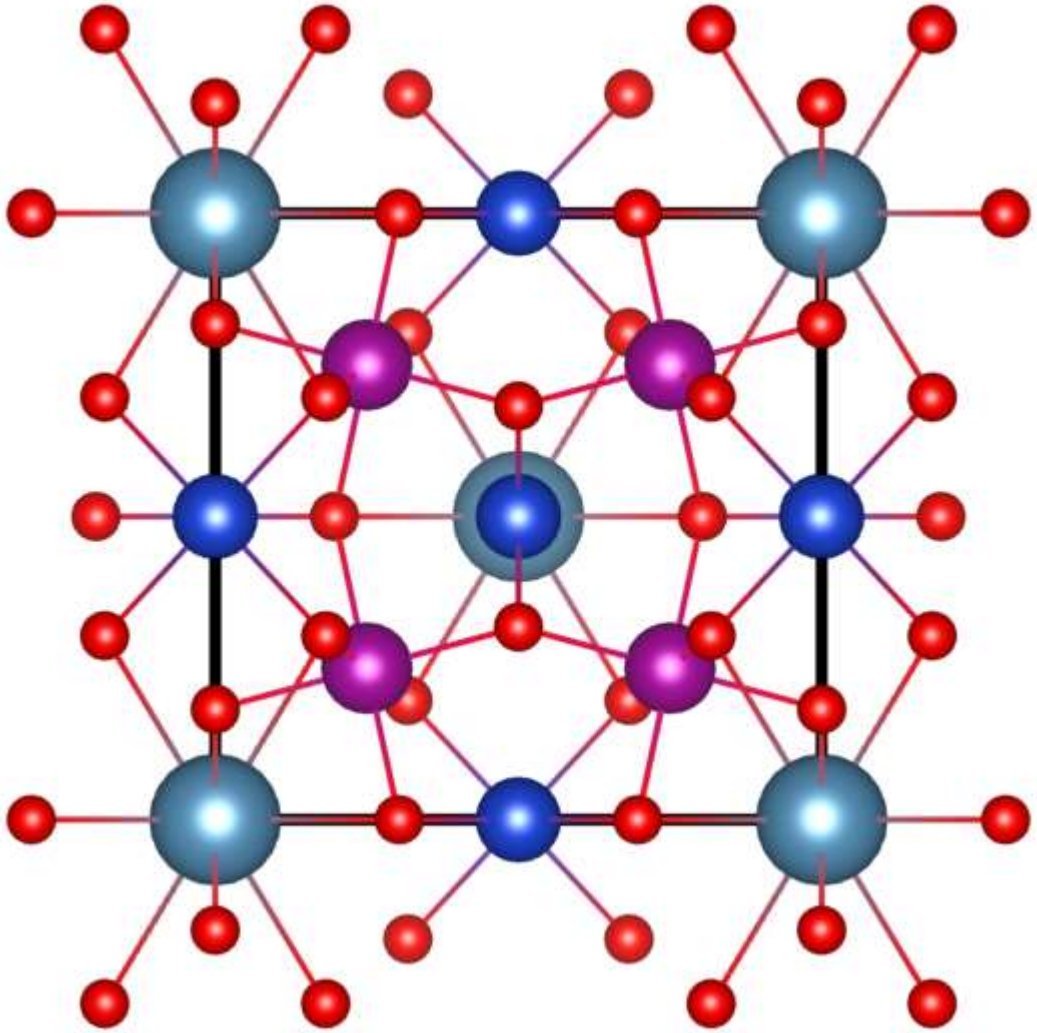
Cube

✓ Equal lengths
✗ Equal angles

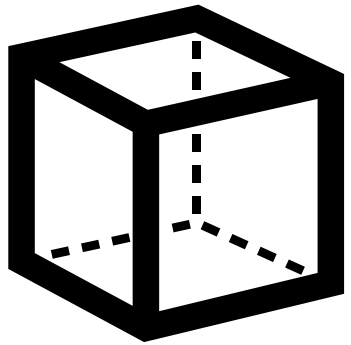


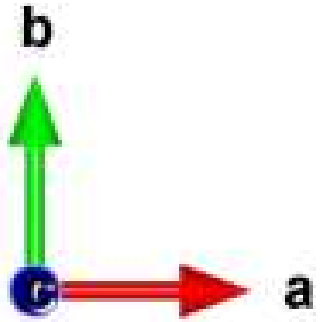
Rhombohedron

Real cubic crystal



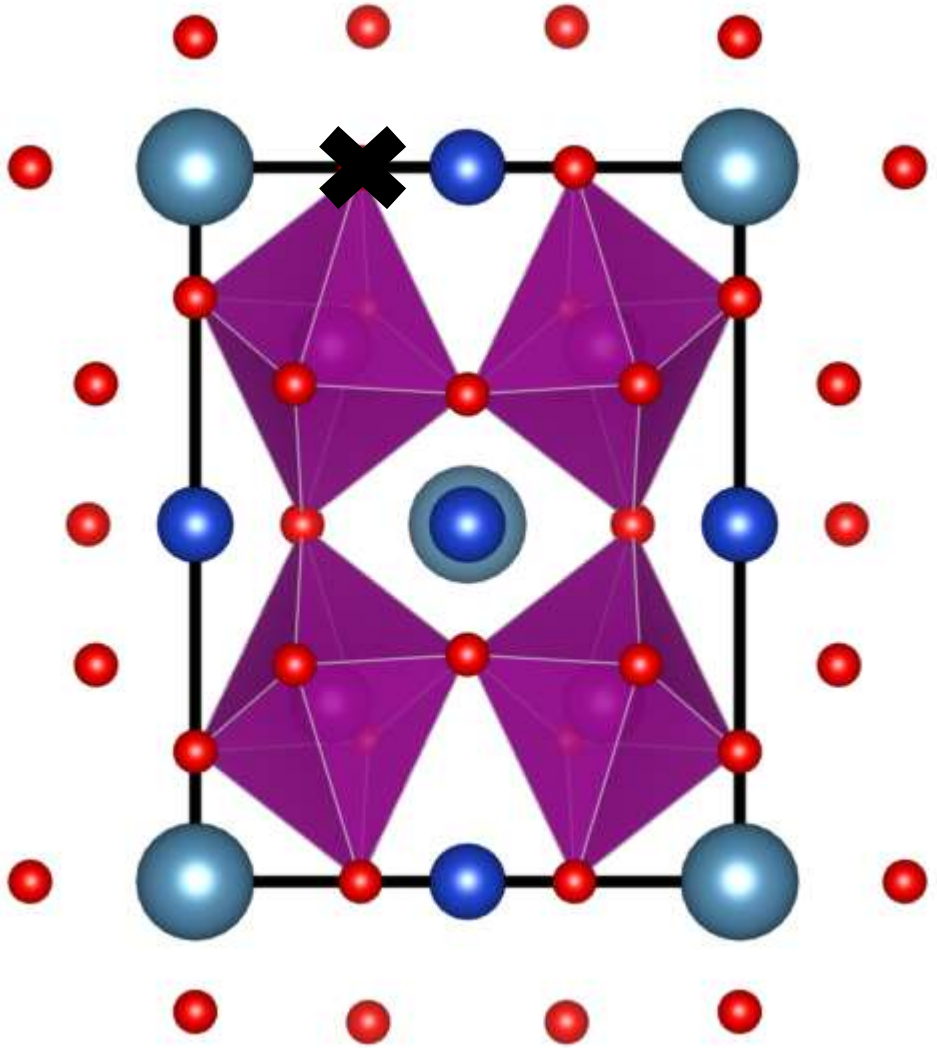
$CaCu_3Mn_4O_{12}$

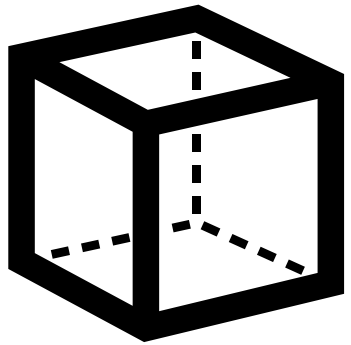


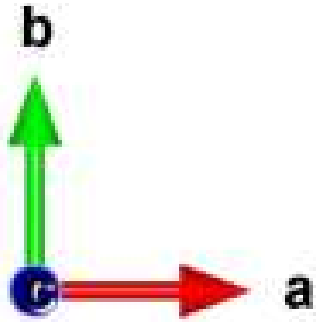


Distortion ⟹ anisotropy

$CaCu_3Mn_4O_{12}$







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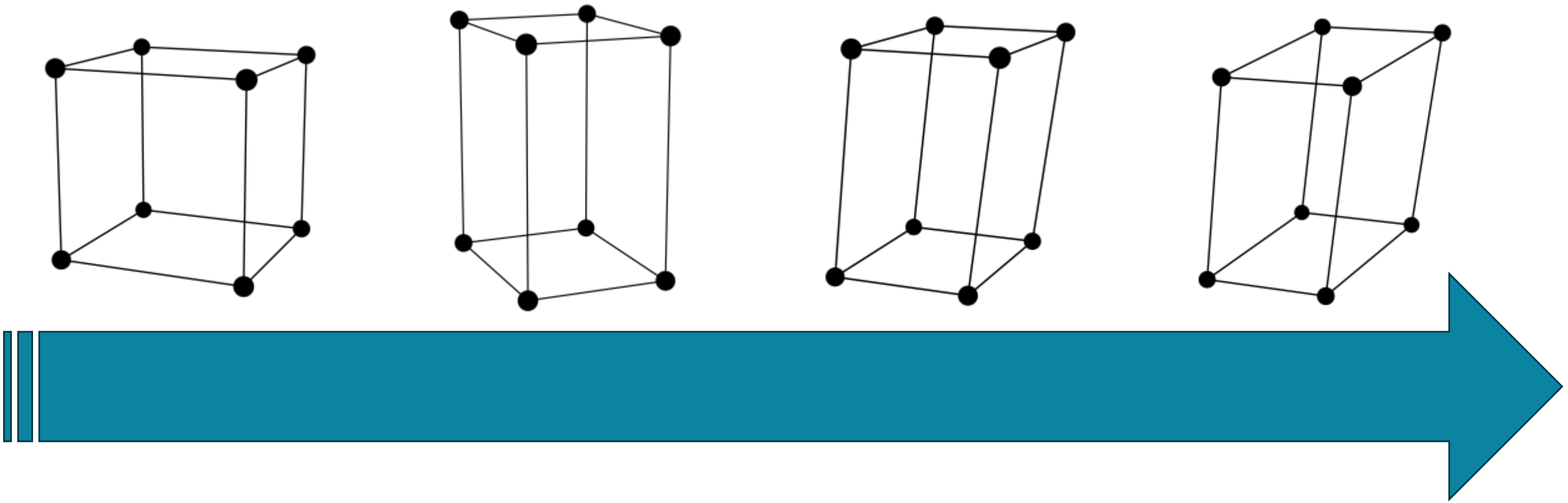
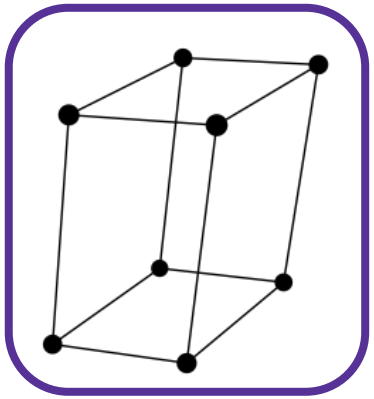
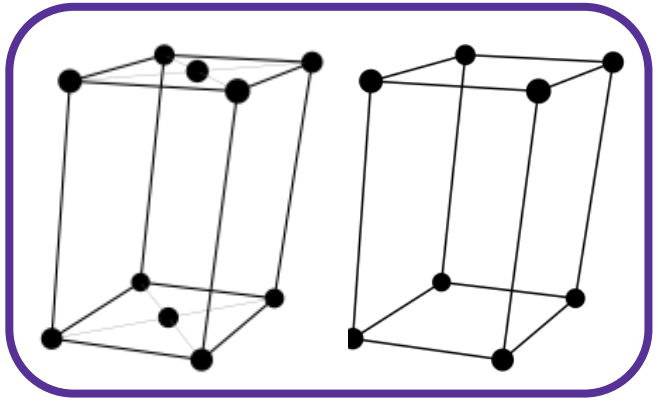
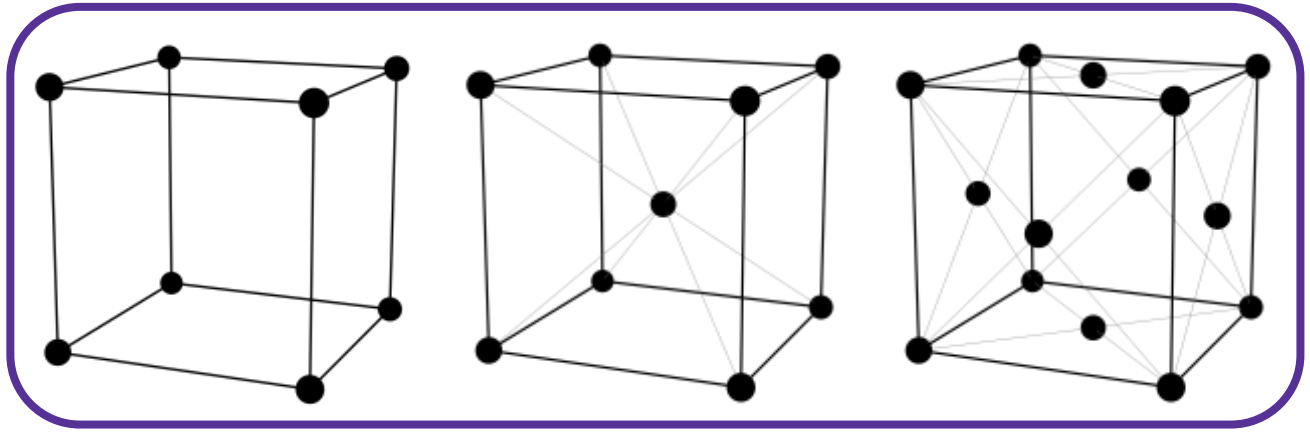
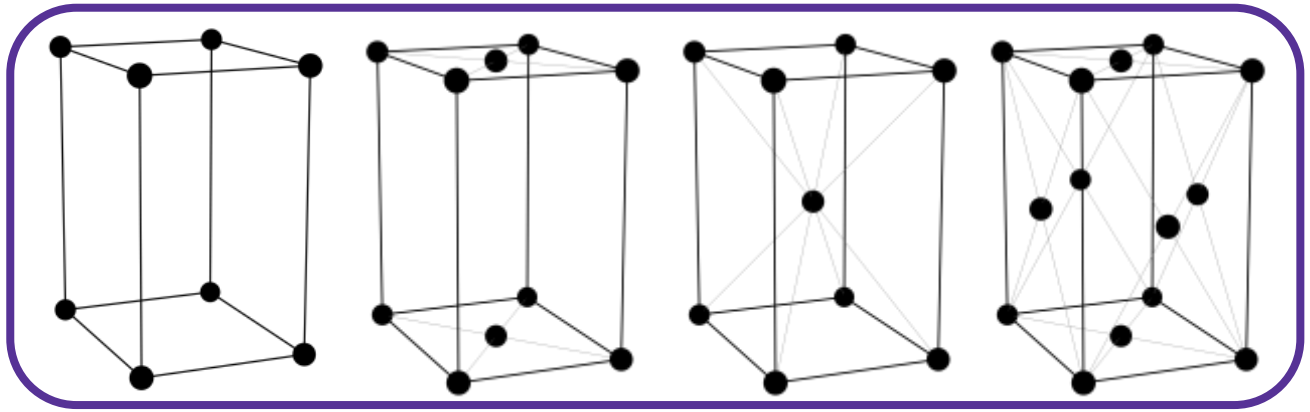
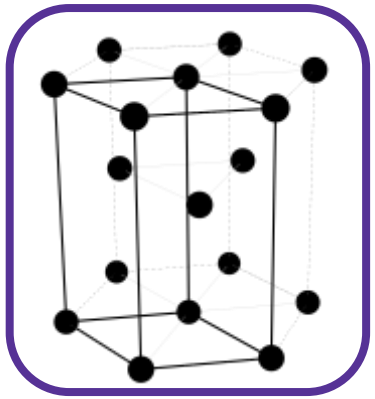
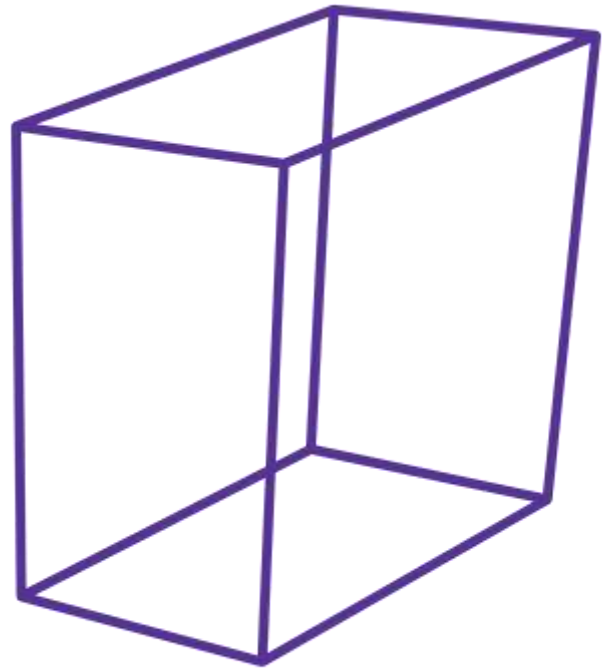
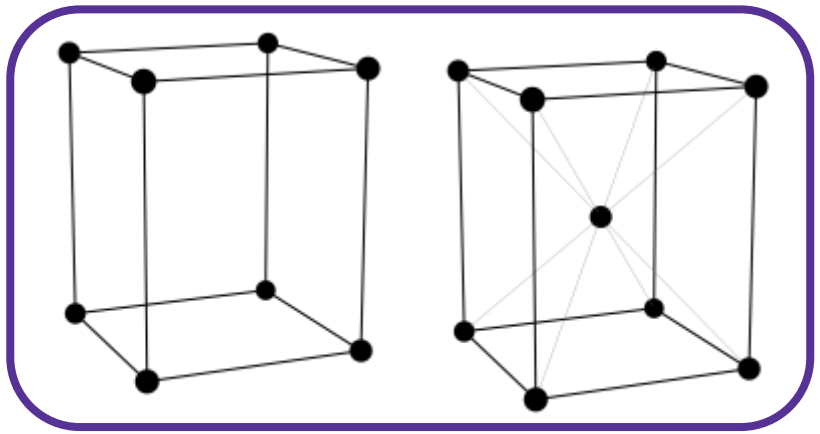
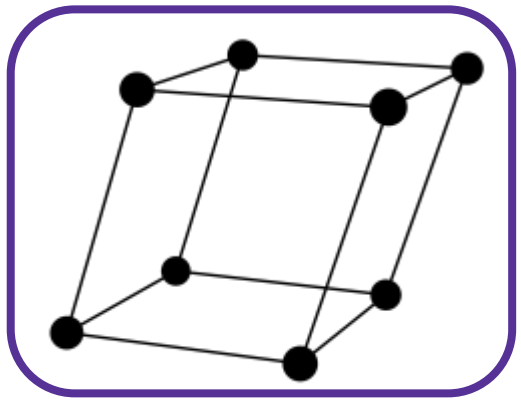
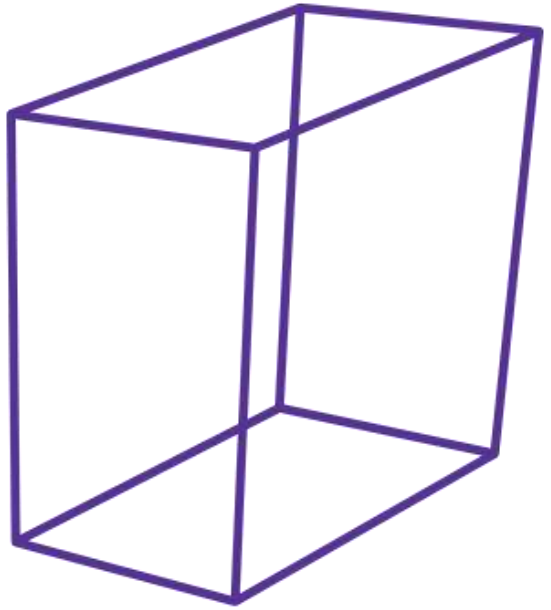


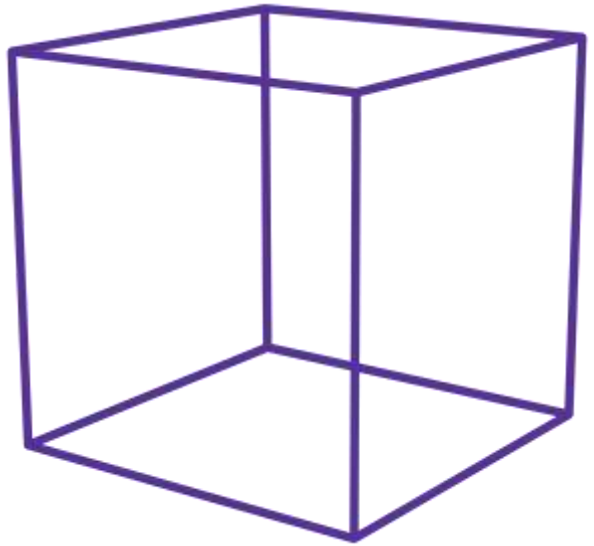









Methodology

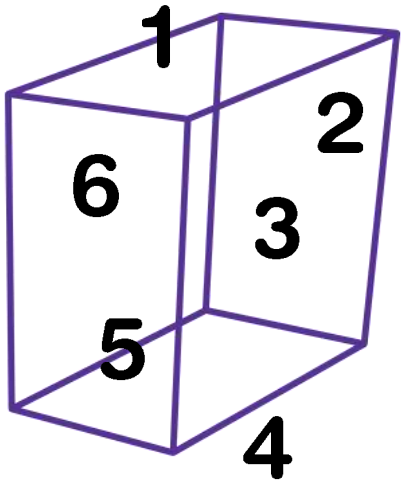
Construct a function which can identify cubic parallelepipeds. It must also be:

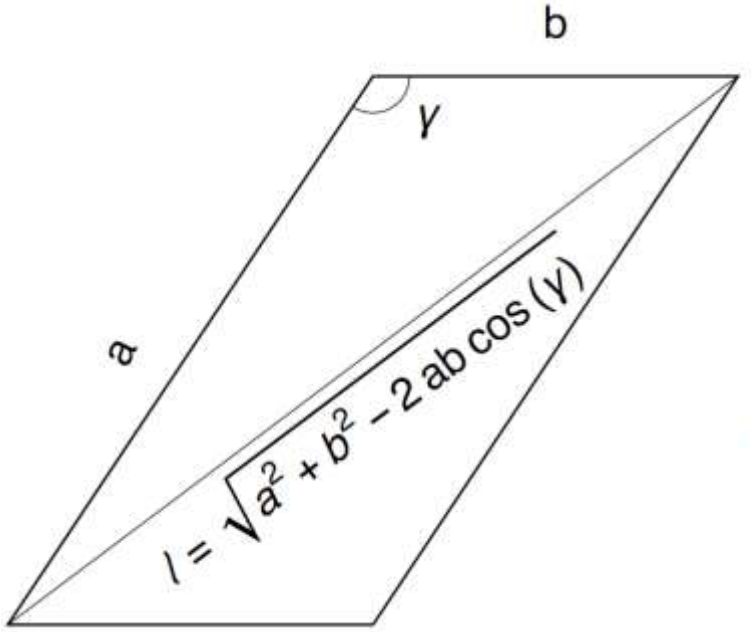
- Dependent on all the lattice parameters only and not on their order
- Volume normalized
- Equal to zero if and only if the shape is a cube
- Display an obvious trend as one lattice parameter is varied

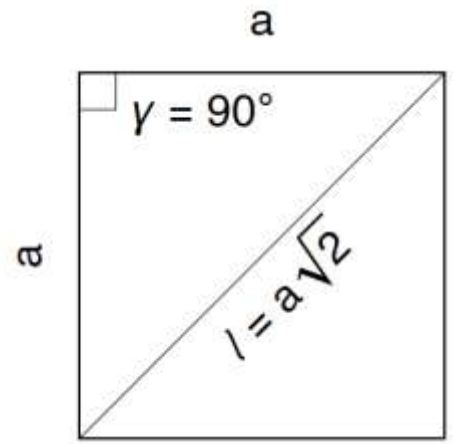




Resulting metric

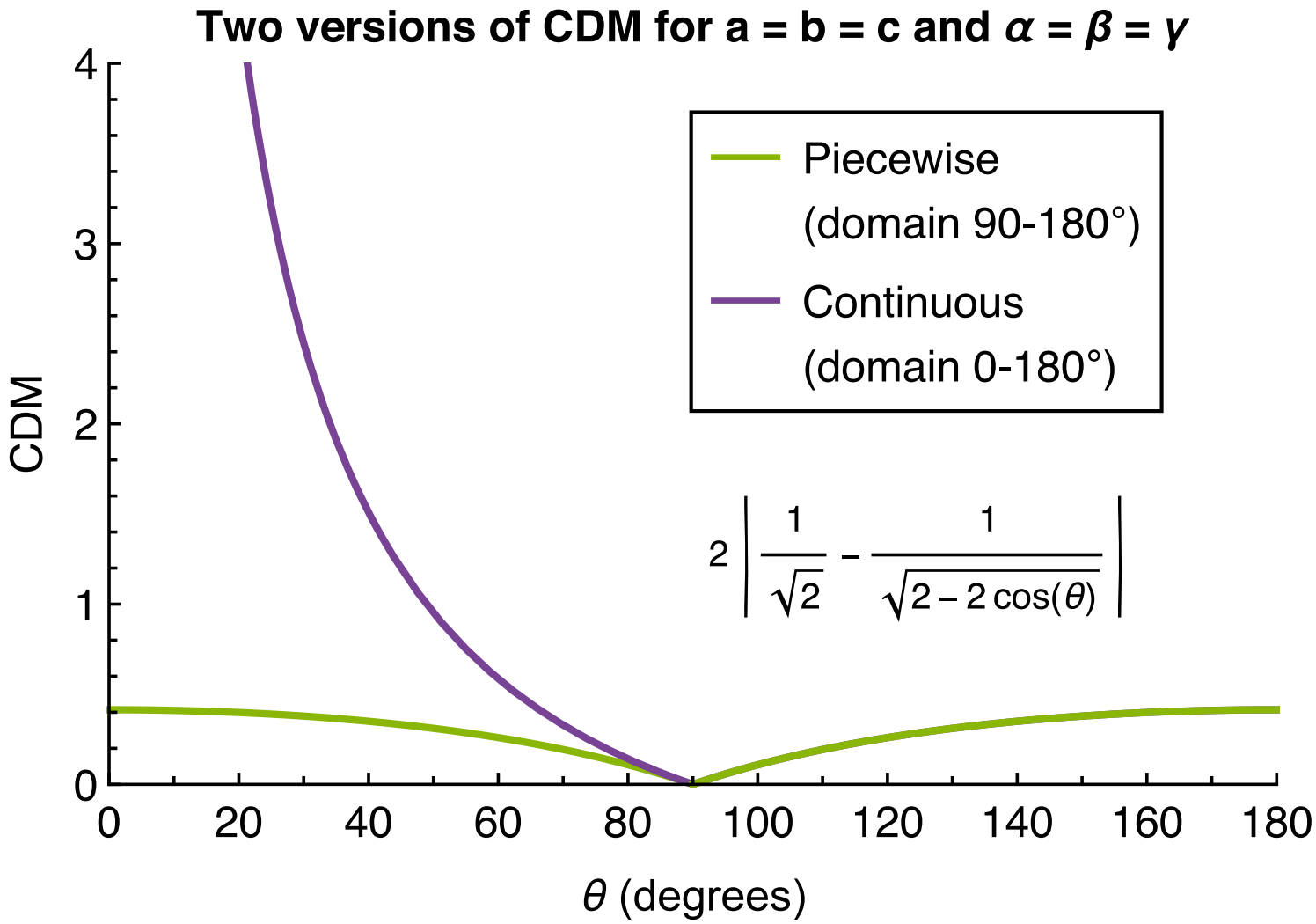






$$\mathcal{M} = \frac{1}{3}\left(\left|\frac{a}{\sqrt{a^2+b^2-2ab\cos(\gamma)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{b}{\sqrt{a^2+b^2-2ab\cos(\gamma)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{c}{\sqrt{a^2+c^2-2ac\cos(\beta)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{a}{\sqrt{a^2+c^2-2ac\cos(\beta)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{b}{\sqrt{b^2+c^2-2bc\cos(\alpha)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{c}{\sqrt{b^2+c^2-2bc\cos(\alpha)}} - \frac{1}{\sqrt{2}}\right|\right)$$

Low angle divergence correction



Piecewise definition

$$\mathcal{M}_{\text{Face AB}} = \begin{cases} \left|\frac{a}{\sqrt{a^2+b^2-2ab\cos(\gamma)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{b}{\sqrt{a^2+b^2-2ab\cos(\gamma)}} - \frac{1}{\sqrt{2}}\right| & \gamma \geq 90° \\ \left|\frac{a}{\sqrt{a^2+b^2-2ab\cos(\gamma-180°)}} - \frac{1}{\sqrt{2}}\right| + \left|\frac{b}{\sqrt{a^2+b^2-2ab\cos(\gamma-180°)}} - \frac{1}{\sqrt{2}}\right| & \gamma < 90° \end{cases}$$

And similar for the remaining two faces, such that:

$$\mathcal{M} = \frac{1}{3}\sum \mathcal{M}_{\text{Face AB}} + \mathcal{M}_{\text{Face BC}} + \mathcal{M}_{\text{Face AC}}$$

Case studies

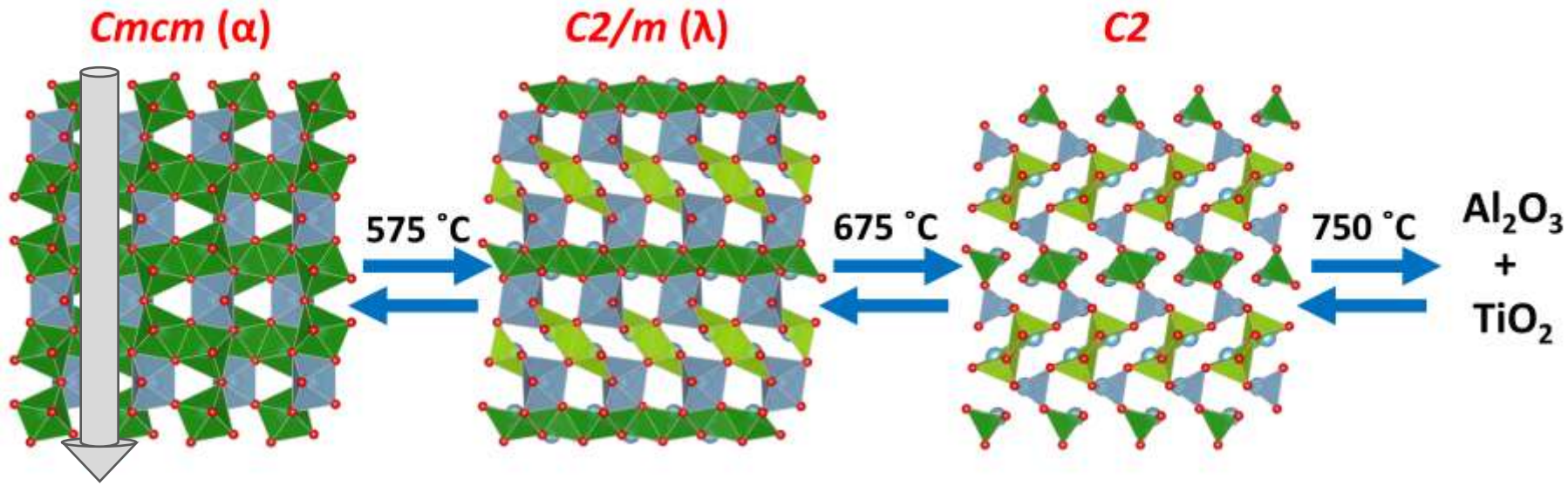
Outline

1. Interpreting phase transitions
2. Comparison to tolerance factors
3. Interpreting structure-driven properties
4. Informing the synthesis of new materials

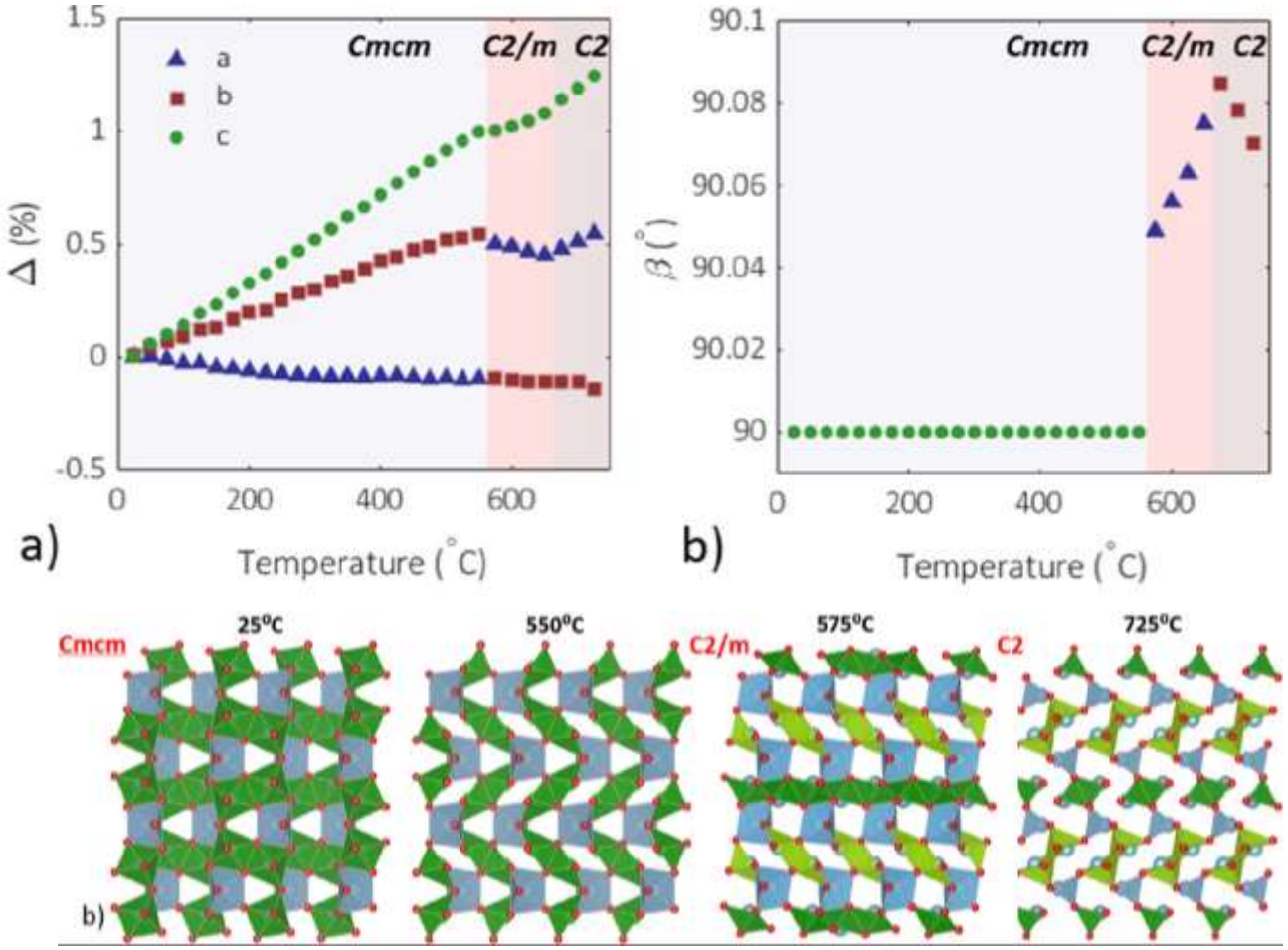
1: Pseudobrookite phases

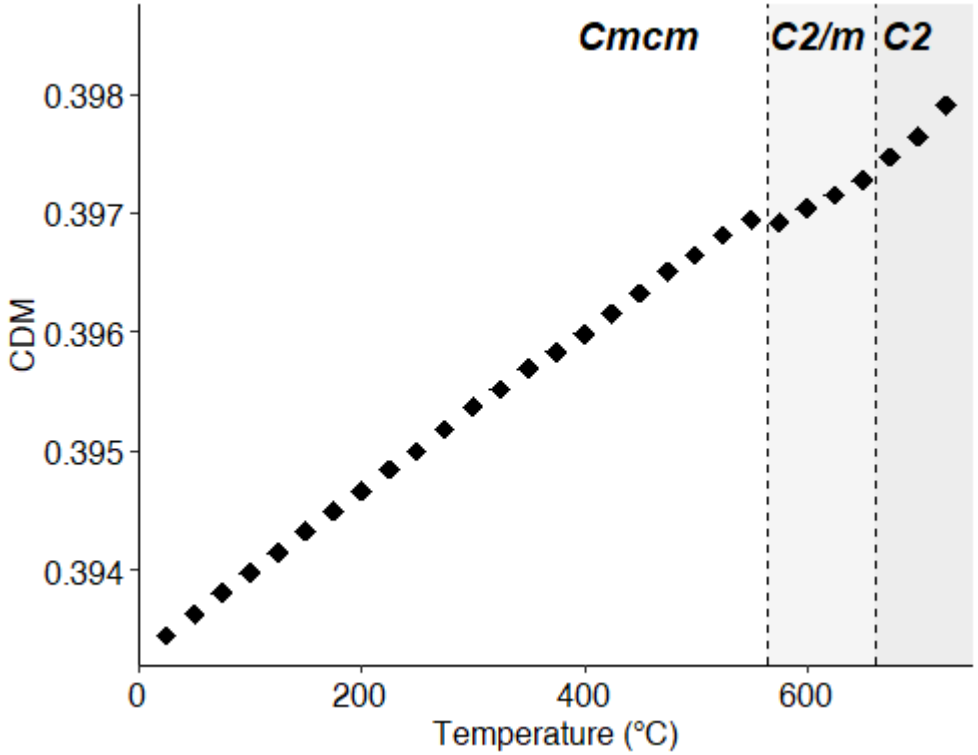
Named for the orthorhombic parent mineral brookite (TiO_2), pseudobrookites are notable for their open channels along the c-axis.

$Al_{2-x}Ti_{1+x}O_5$



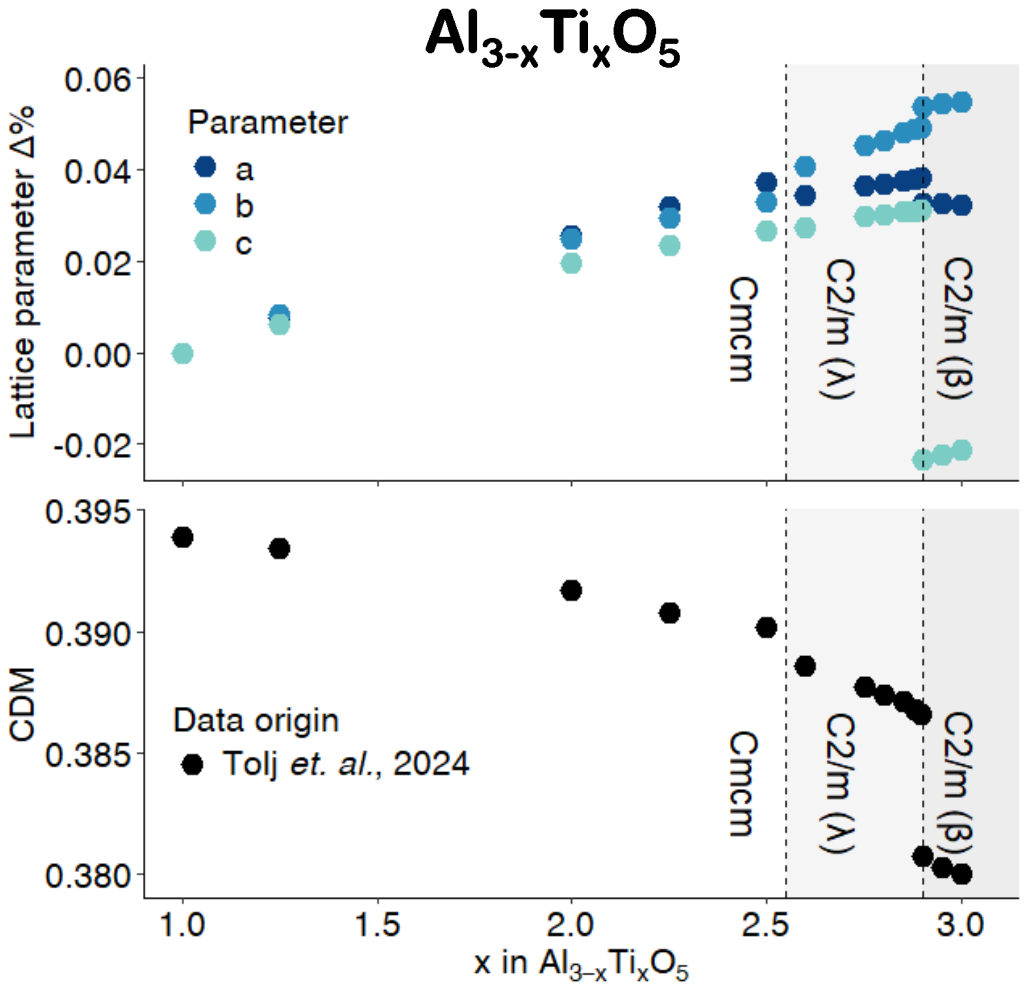
Origin choices resolved

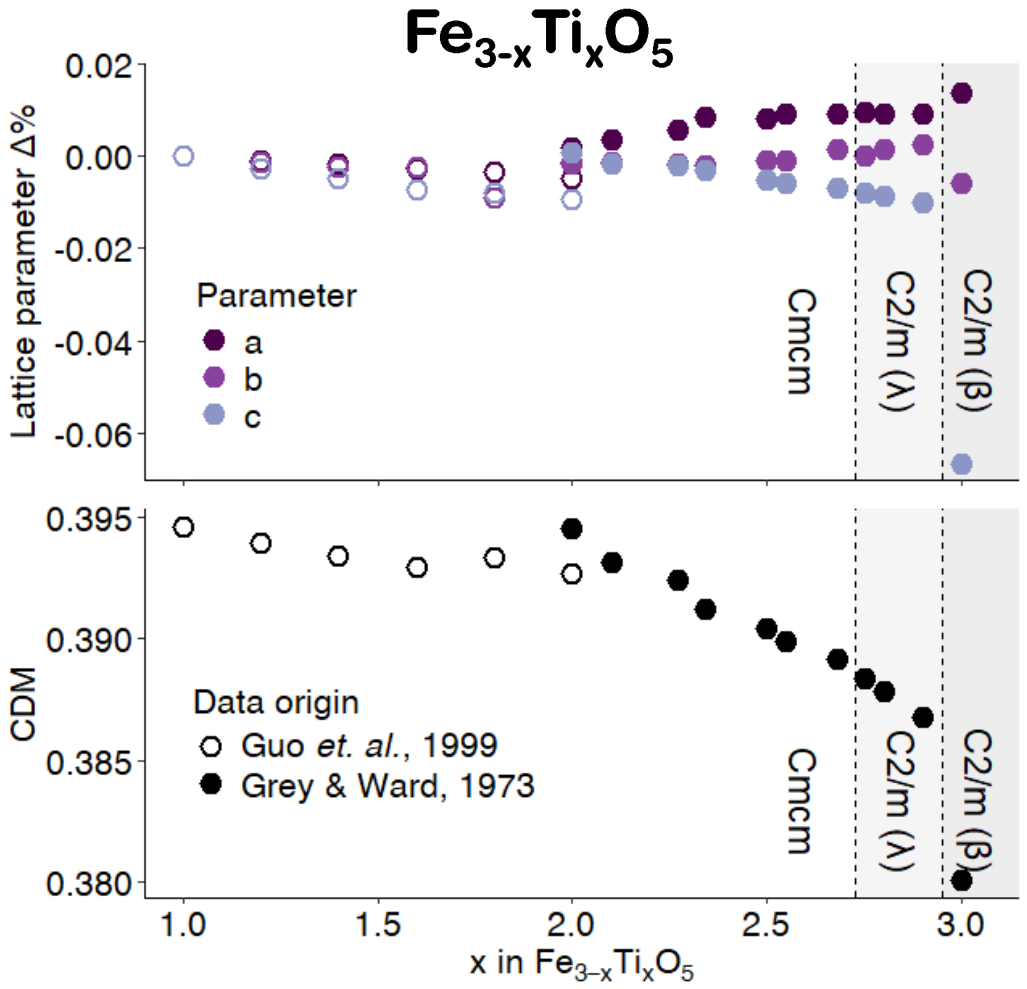




Cryst. Growth Des. 2024, 24, 2, 688–695

Clearer comparisons

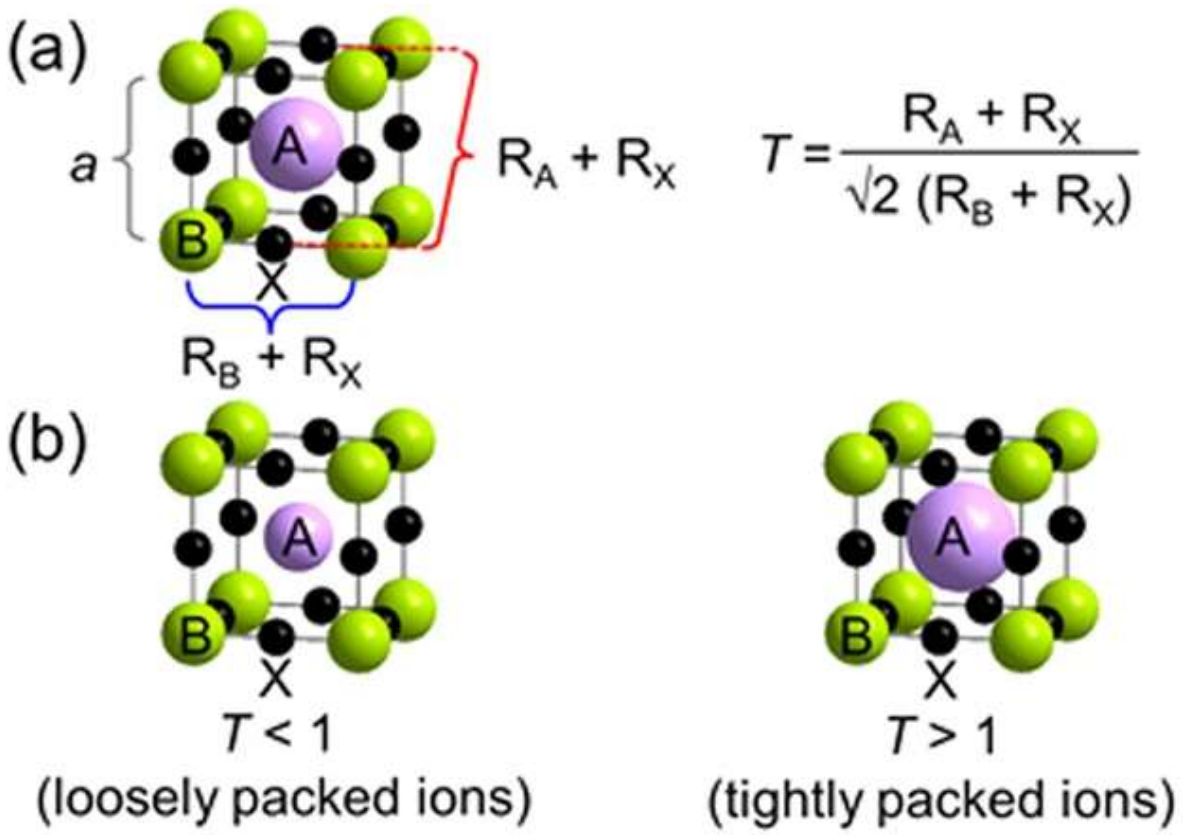




Cryst. Growth Des. 2024, 24, 2, 688–695

J. Phys.: Condens. Matter 1999, 11, 6337-6346
J. Solid State Chem. 1973, 7, 300-307

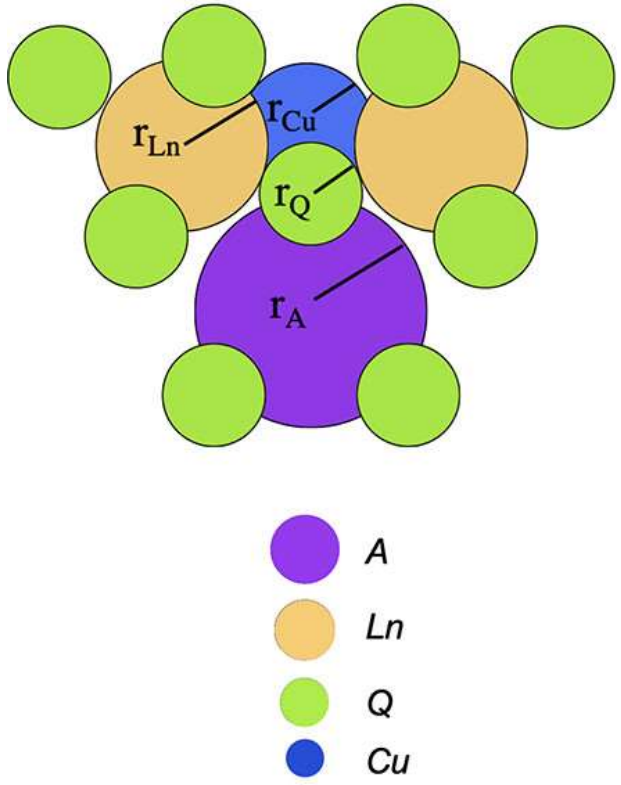
2: Homologies & tolerance factors

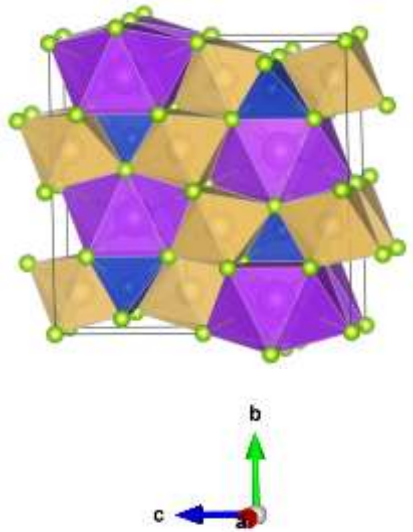


- STFs can predict the stability of new phases *before* synthesis requiring only ionic radii.
- Structural homologies follow trends dependent on ionic radii, and therefore tolerance factors also show trends.

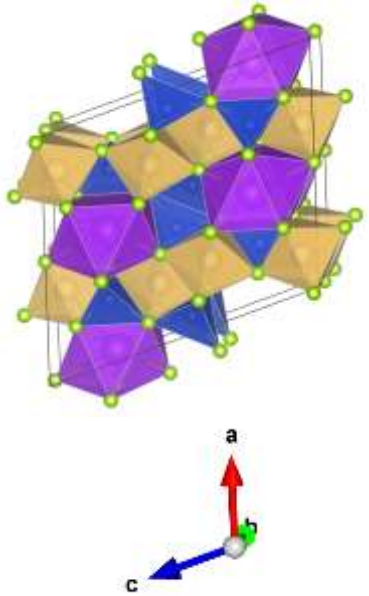
Sci Rep 2016, 6, 23592

Quaternary tolerance factor

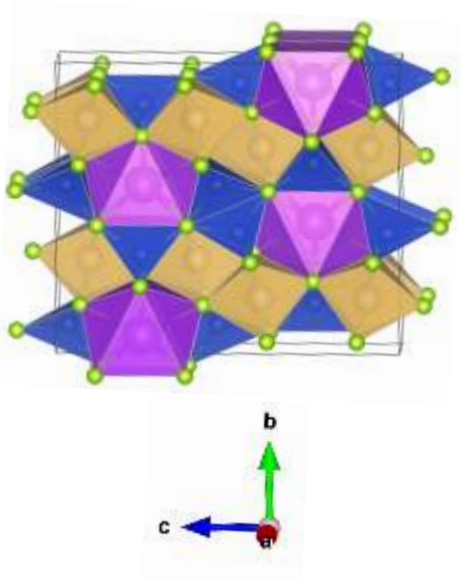




ALn_2CuQ_4
n = 1 *Cmcm*



$A_2Ln_4Cu_4Q_9$
n = 2 *C2/m*



$ALn_2Cu_3Q_5$
n = 3 *Cmcm*

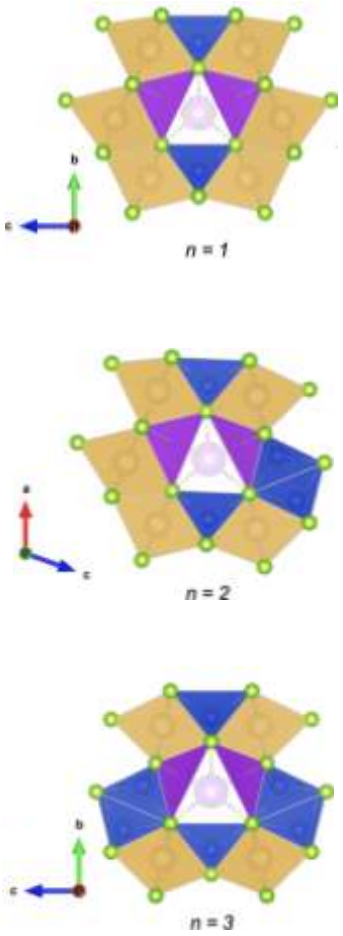
$A_2Ln_4Cu_{2n}Q_{7+n}$

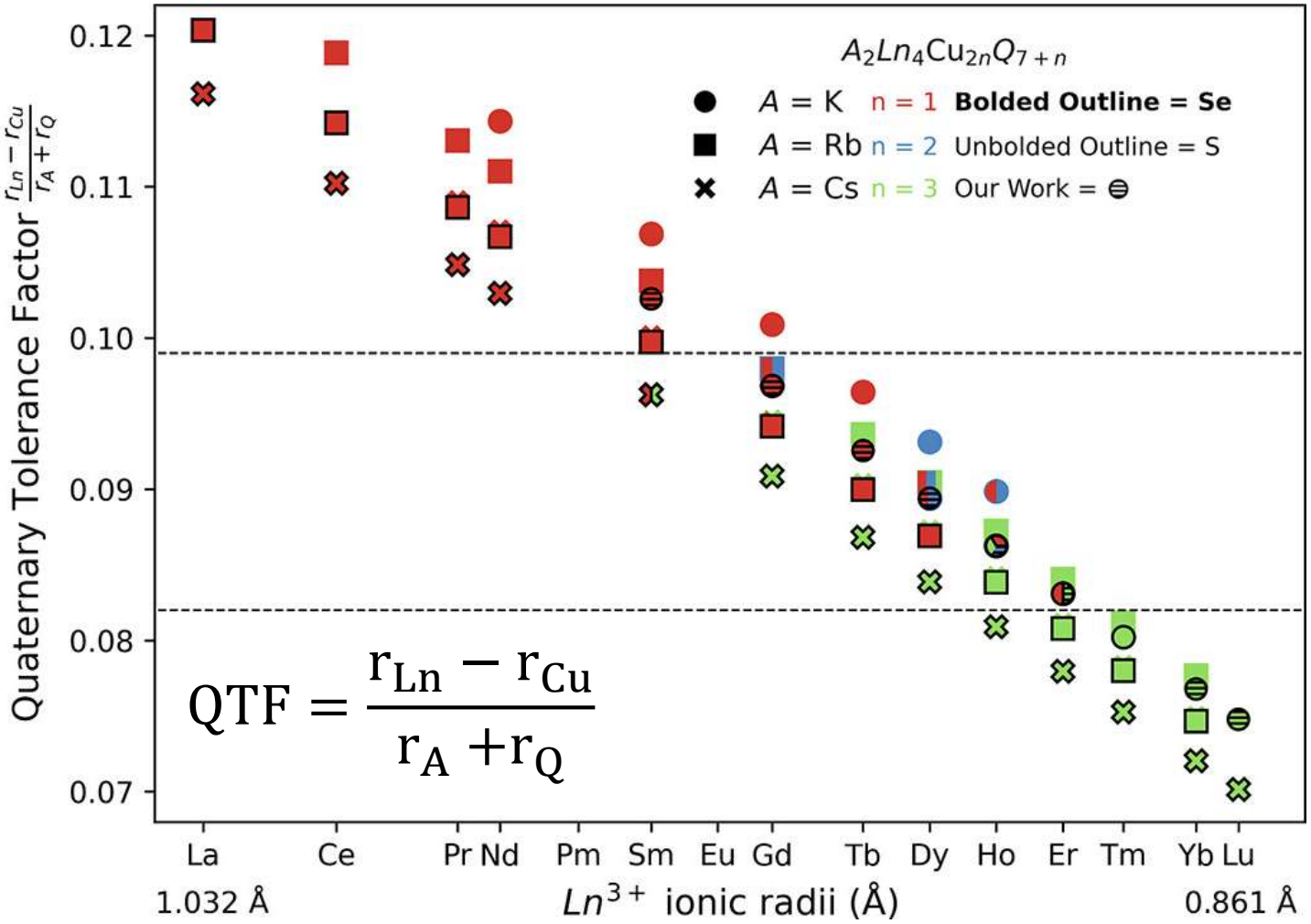
$$QTF = \frac{r_{Ln} - r_{Cu}}{r_A + r_Q}$$

J. Am. Chem. Soc. 2024, 146, 36, 25190-25199

QTF trends

A
Ln
Cu
Q





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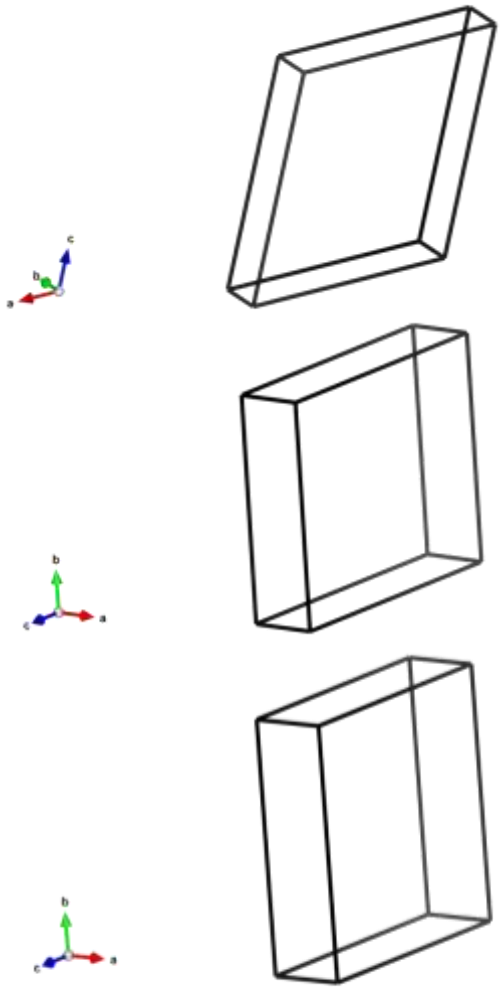
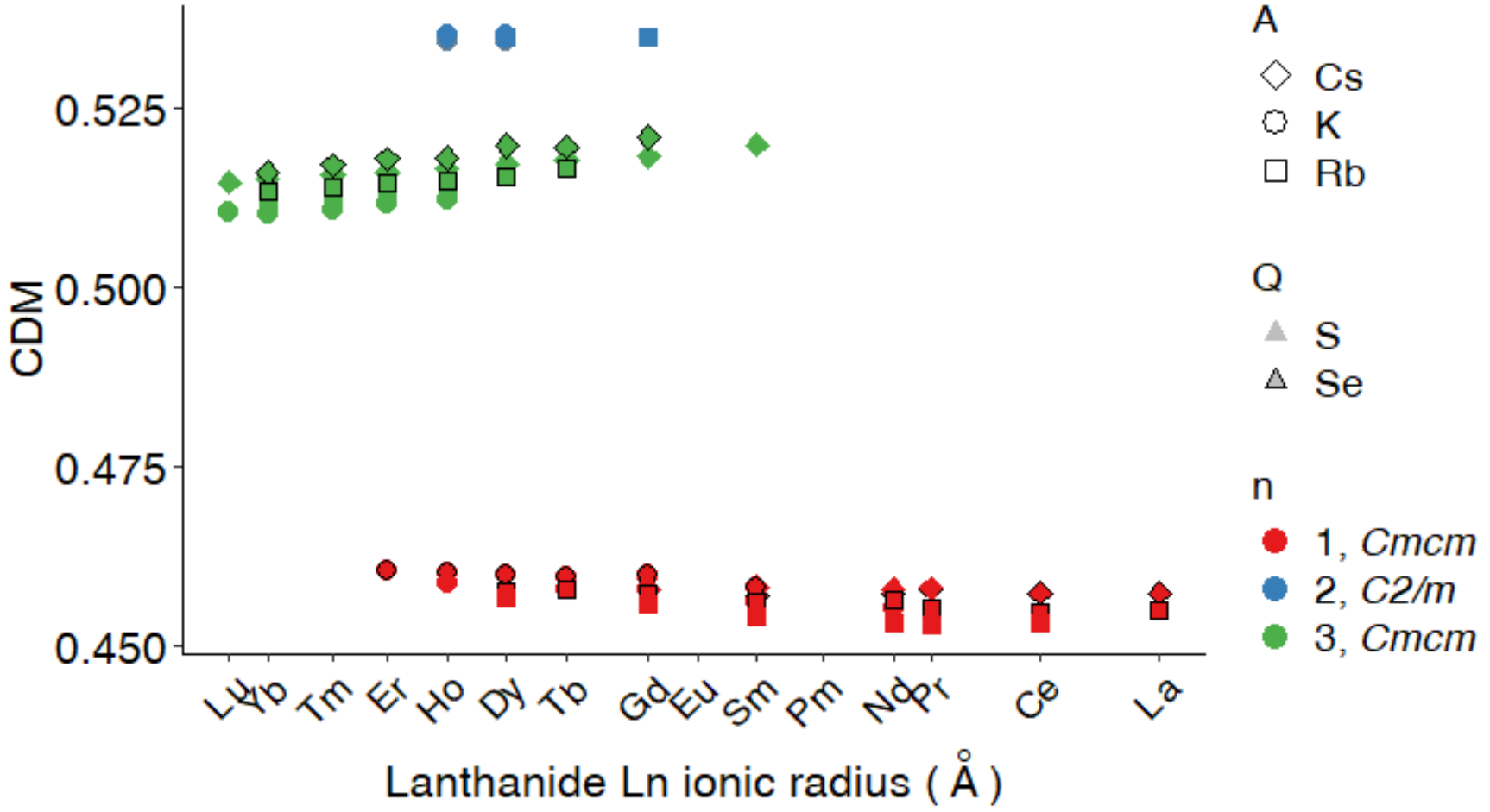
J. Am. Chem. Soc. 2024, 146, 36, 25190-25199

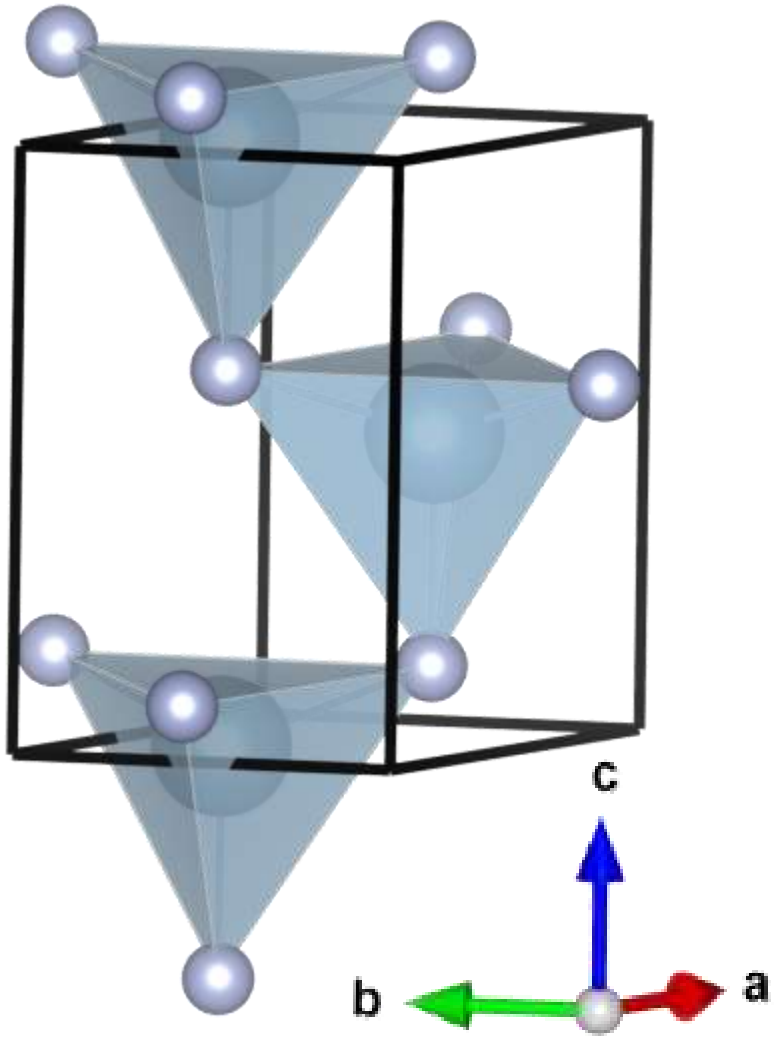
CDM separates trends





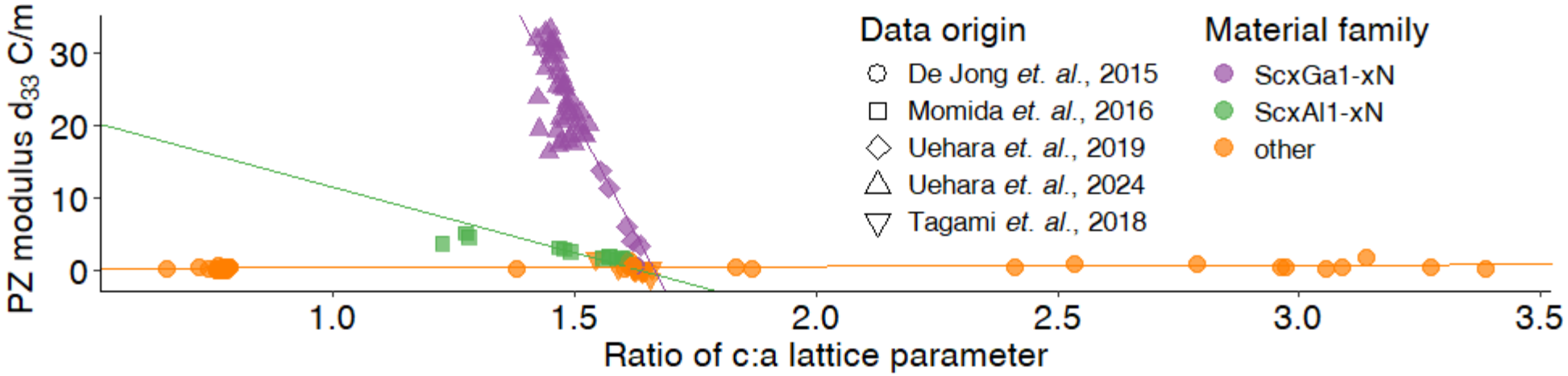
J. Am. Chem. Soc. 2024, 146, 36, 25190-25199

3: Piezoelectric materials



- The piezoelectric modulus d_{33} quantifies volume change under applied electric field.
- In the Wurtzite crystal structure, the change is driven by cation-anion separation along the c-axis.
- Theory and experiment agree that the ratio of c:a lengths in Wurtzites correlates with d_{33}.

Known d_{33} trend



Scientific Data 2015, 2, 150053

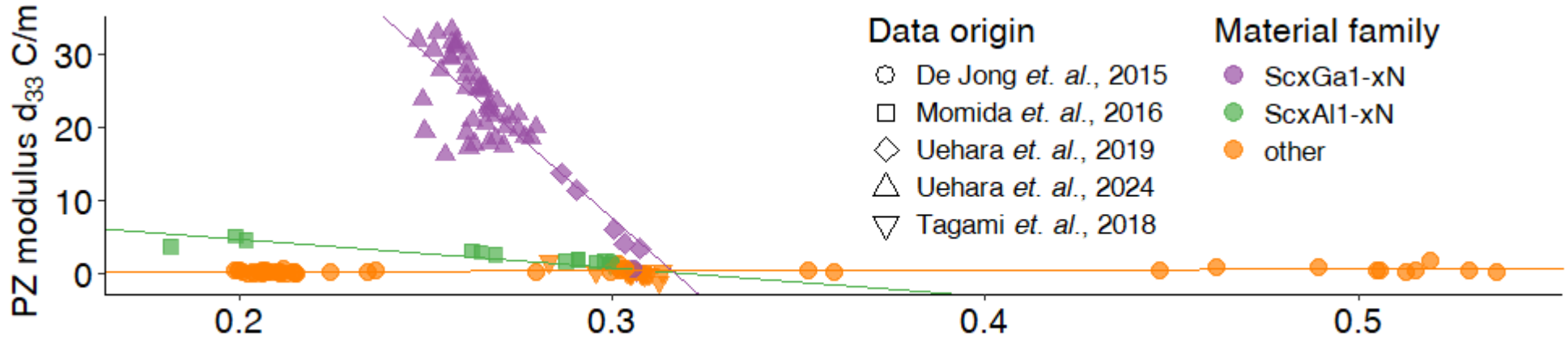
AIP Advances 2016, 6, 065006

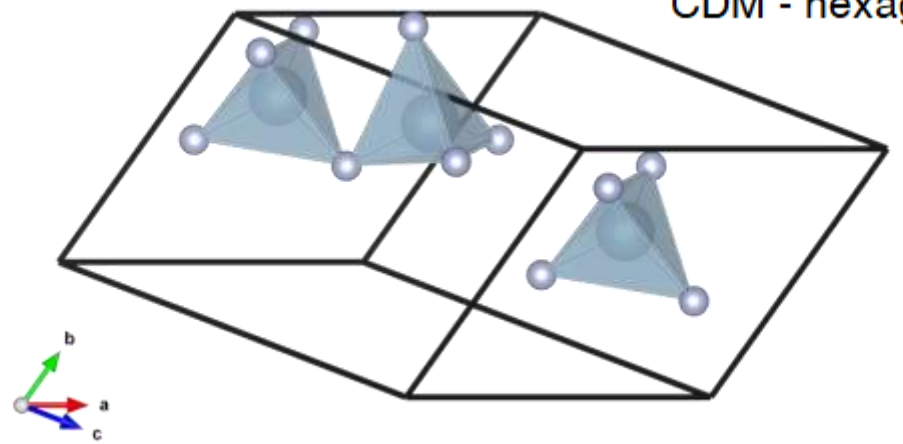
Appl. Phys. Lett. 2019, 114, 012902

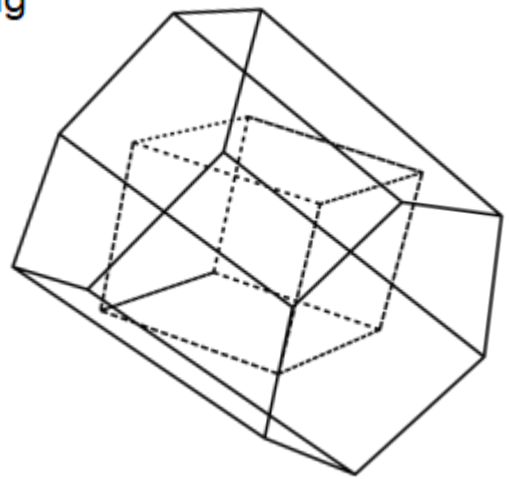
APL Mater. 2024, 12, 121102

Appl. Phys. Express 2018, 11, 041201

CDM replicates known trend



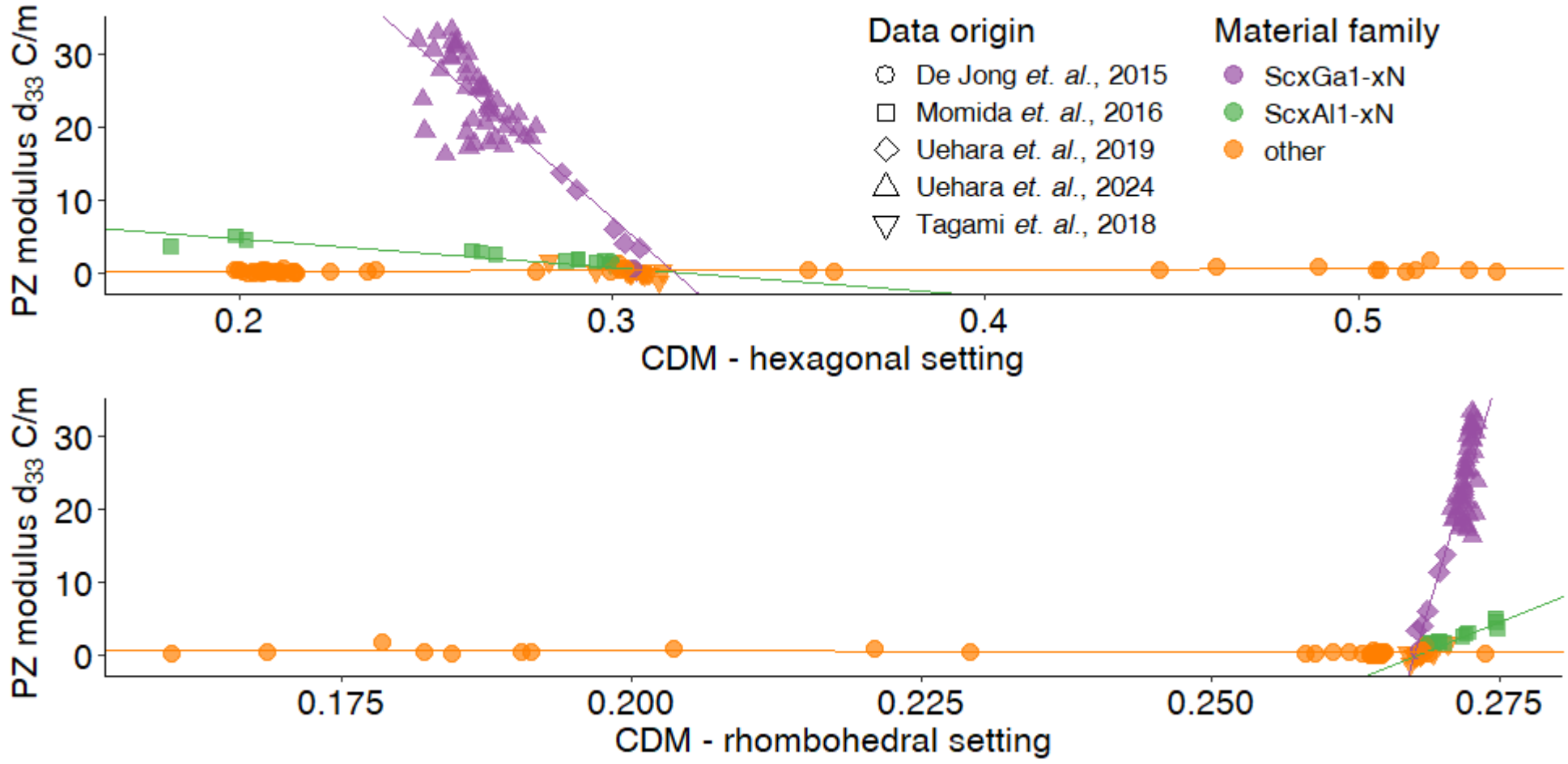




D-cell

Scientific Data 2015, 2, 150053
AIP Advances 2016, 6, 065006
Appl. Phys. Lett. 2019, 114, 012902
APL Mater. 2024, 12, 121102
Appl. Phys. Express 2018, 11, 041201

CDM replicates known trend



Scientific Data 2015, 2, 150053

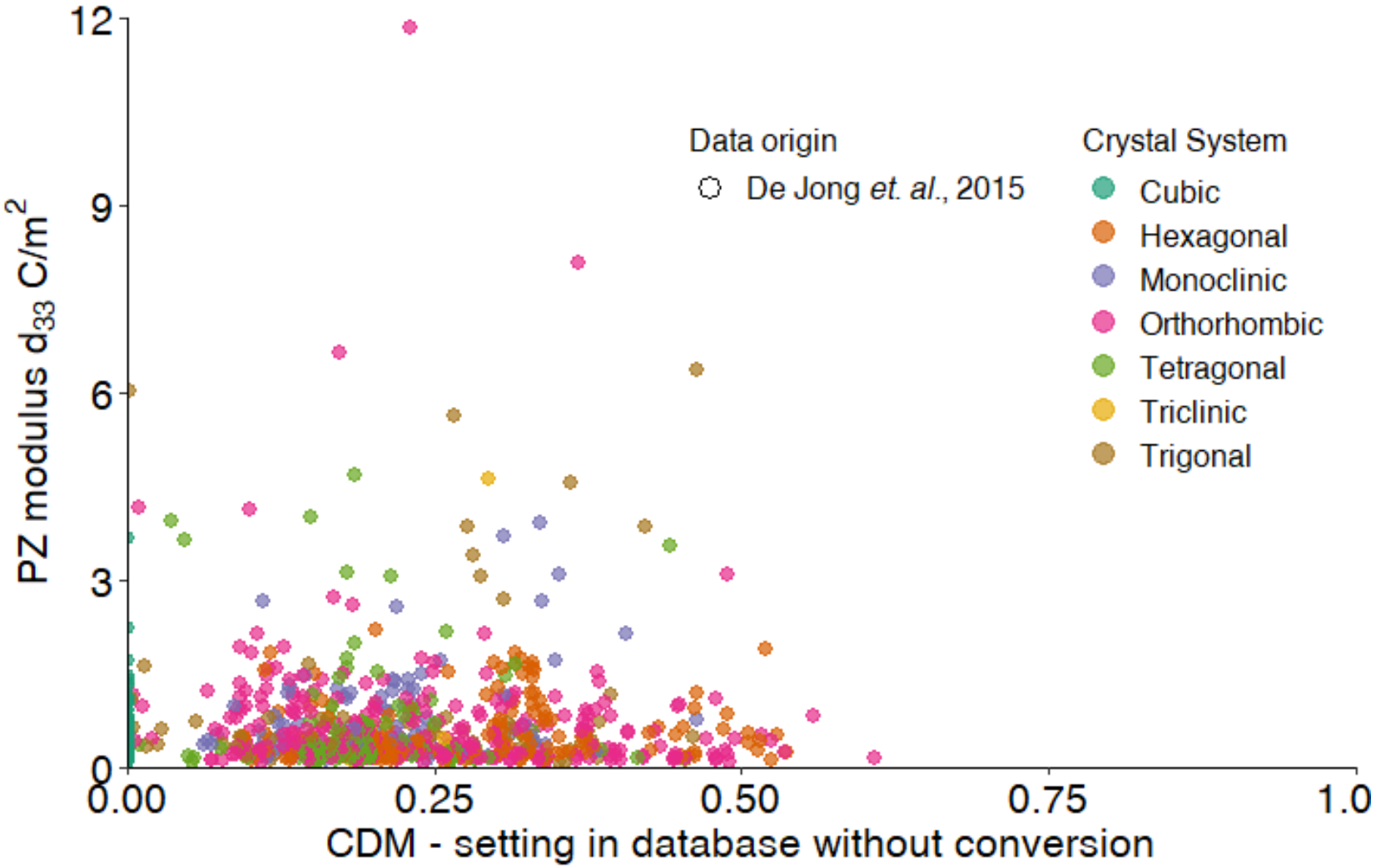
AIP Advances 2016, 6, 065006

Appl. Phys. Lett. 2019, 114, 012902

APL Mater. 2024, 12, 121102

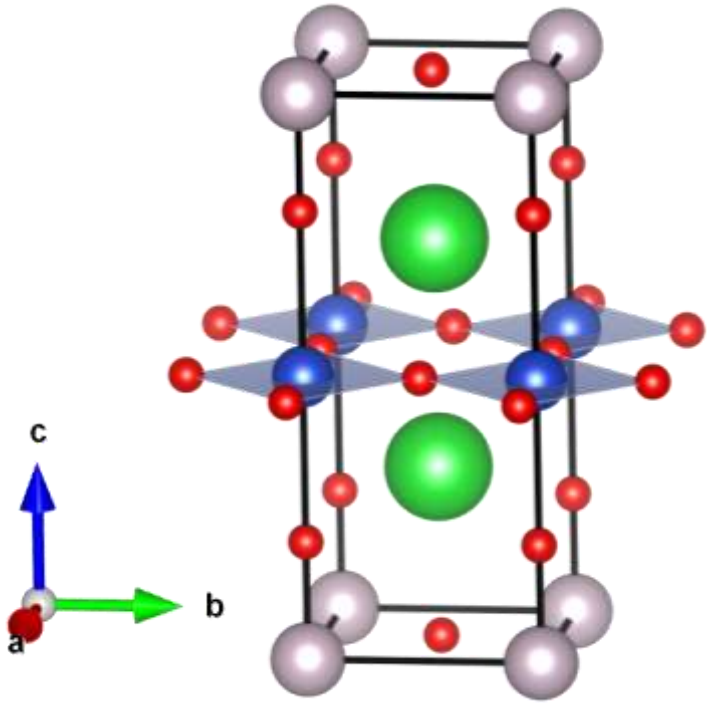
Appl. Phys. Express 2018, 11, 041201

Possible applications?

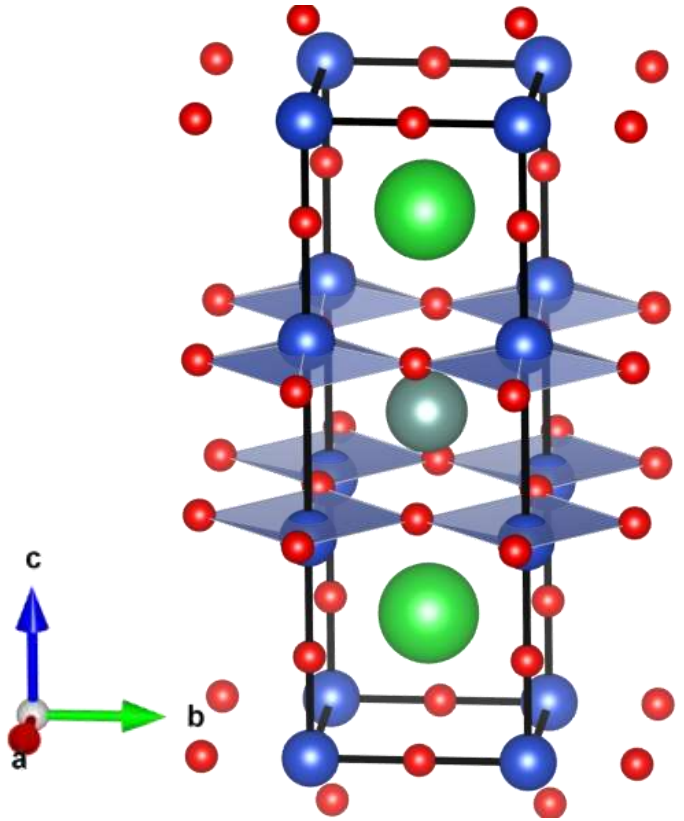


Scientific Data 2015, 2, 150053

4: Cuprate chemistry



$HgBa_2CuO_4$



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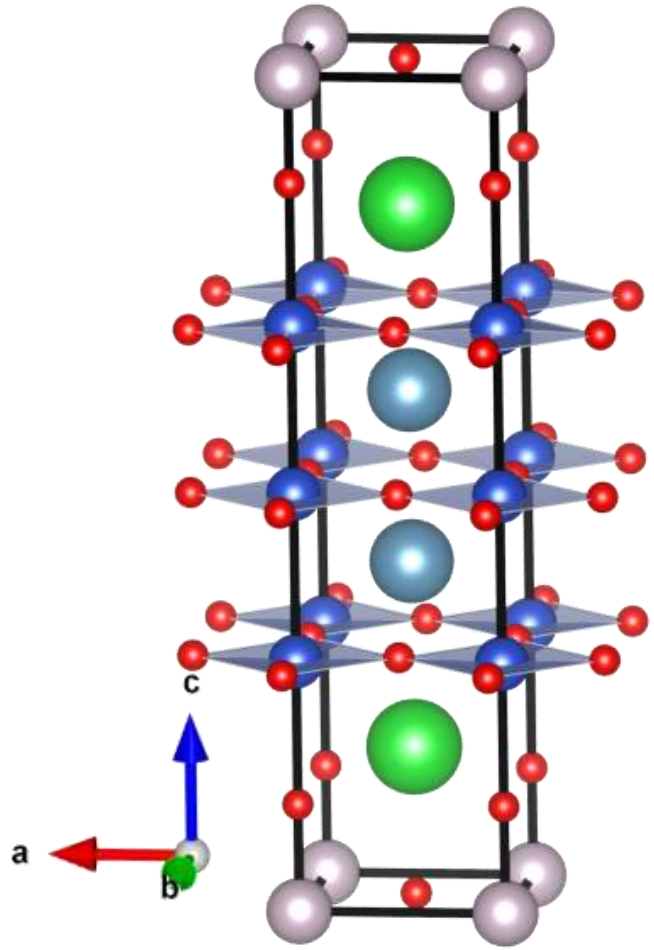
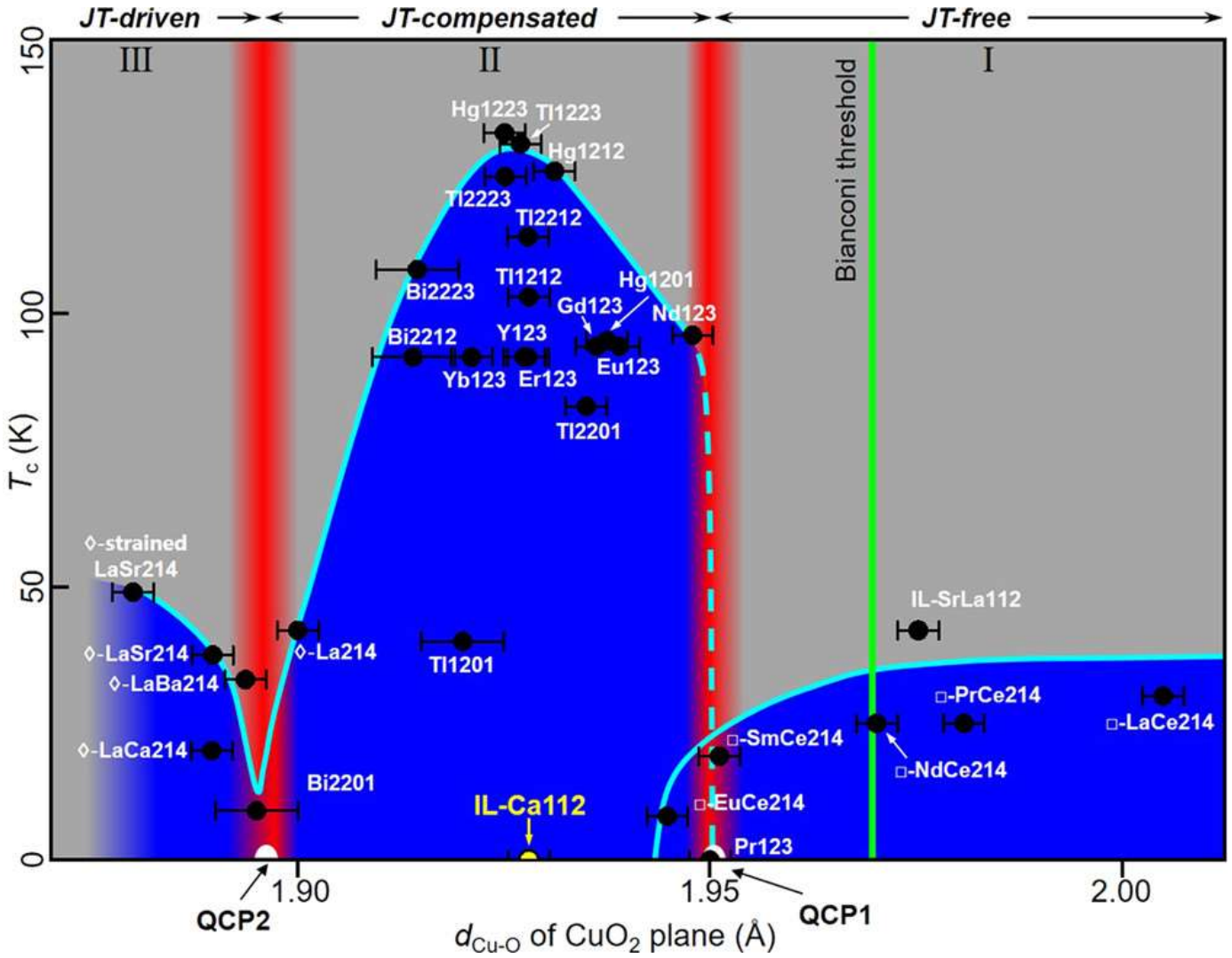


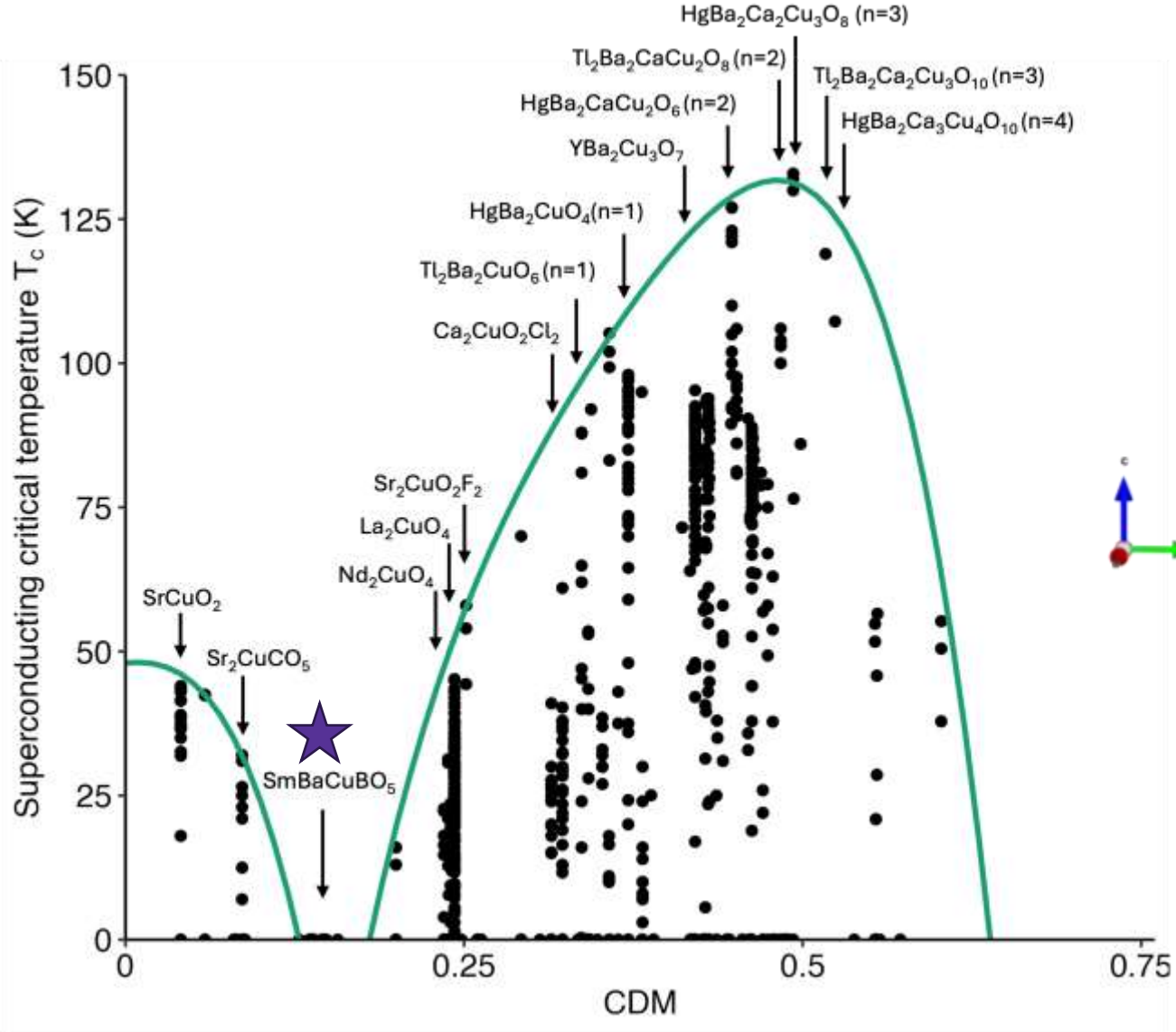
$HgBa_2Ca_2Cu_3O_8$

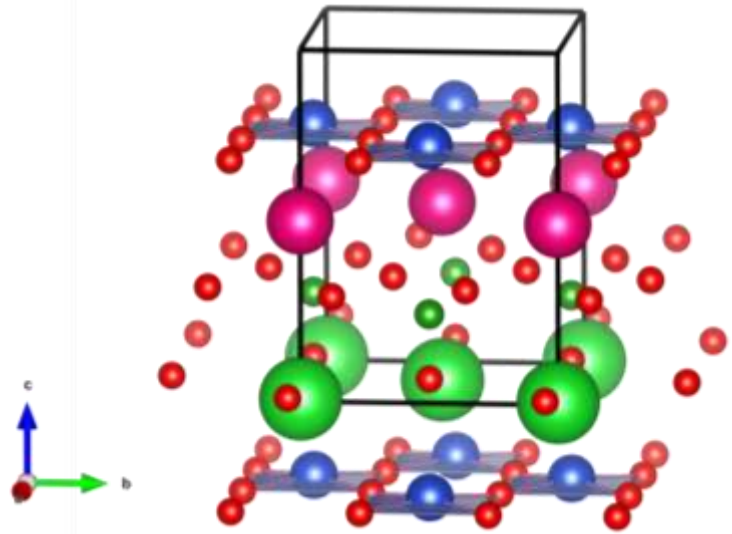
Superconductivity "domes"



ACS Omega 2021, 6, 34, 21884–21891

CDM suggests new candidates





$SmBa_2CuBO_5$

Scientific Data 2023, 10, 816

Conclusions & future work

- A volume-normalized tool called the CDM was developed for application to all 7 crystal systems.
  - This tool acts as a quantitative descriptor to be used alongside words such as “pseudocubic”.
- The CDM is best suited for post-synthesis analysis, but can inform materials design.
- Future work includes such as applications as mixed-phase systems (solid solutions) and more rigorous mathematical investigation of its limits

Links to our work

Our paper in progress

CDM implementation

Comparison to similar tools