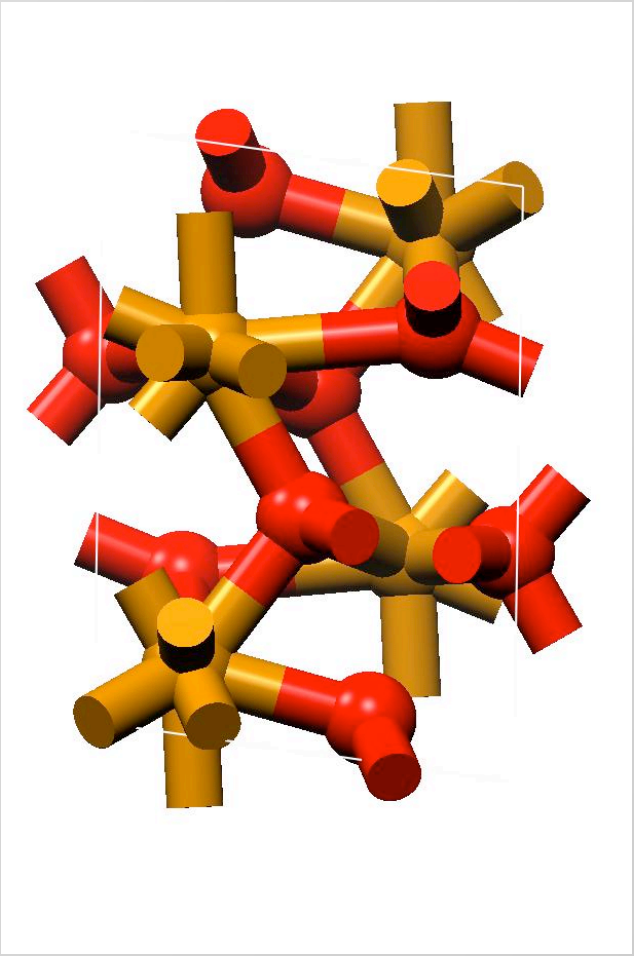
Post-Cotunnite Phase of TeO_2



Phys. Rev. B 72, 092101 (2005)
Post- $PbCl_2$ phase transformation of TeO_2

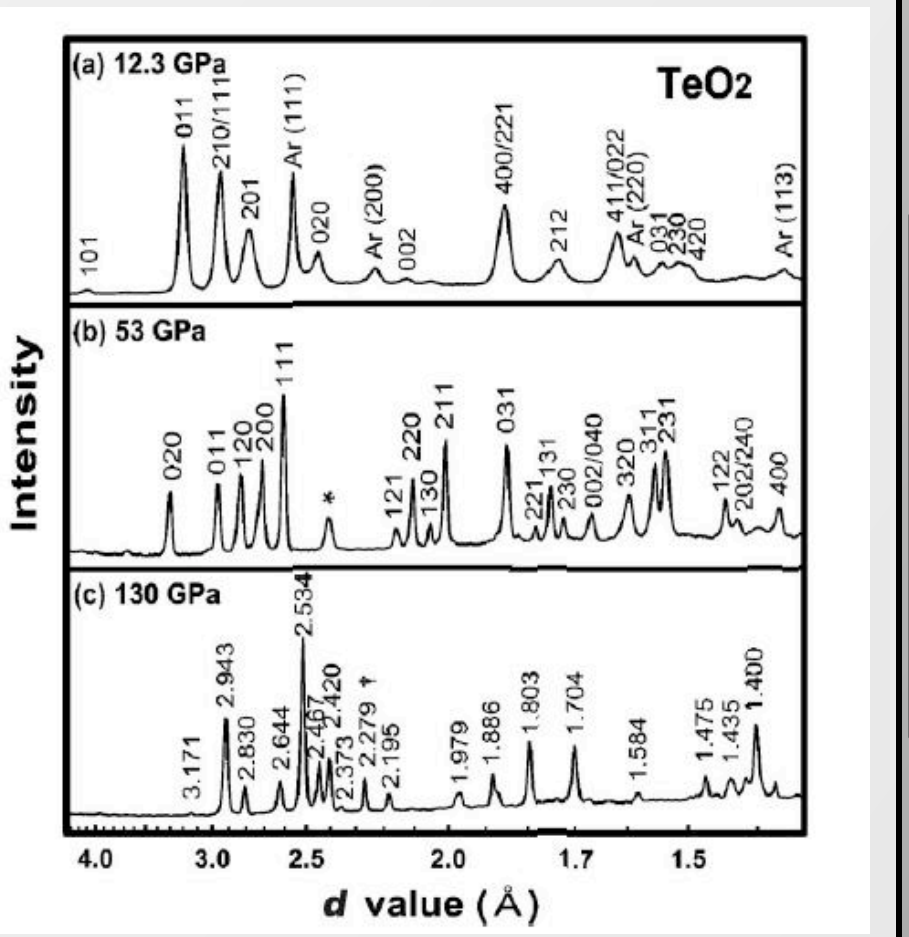
Tomoko Sato, Nobumasa Funamori, Takehiko Yagi, and Nobuyoshi Miyajima

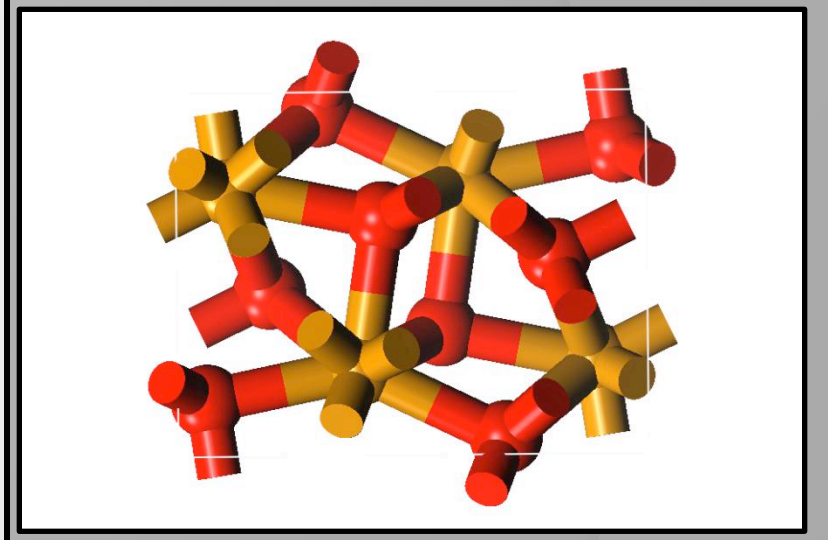
Submitted to Phys. Rev. B (June 2009)
Post- Cotunnite phase of TeO_2

http://arxiv.org/abs/0906.4467

Gareth I. G. Griffiths, Chris J. Pickard, and R. J. Needs

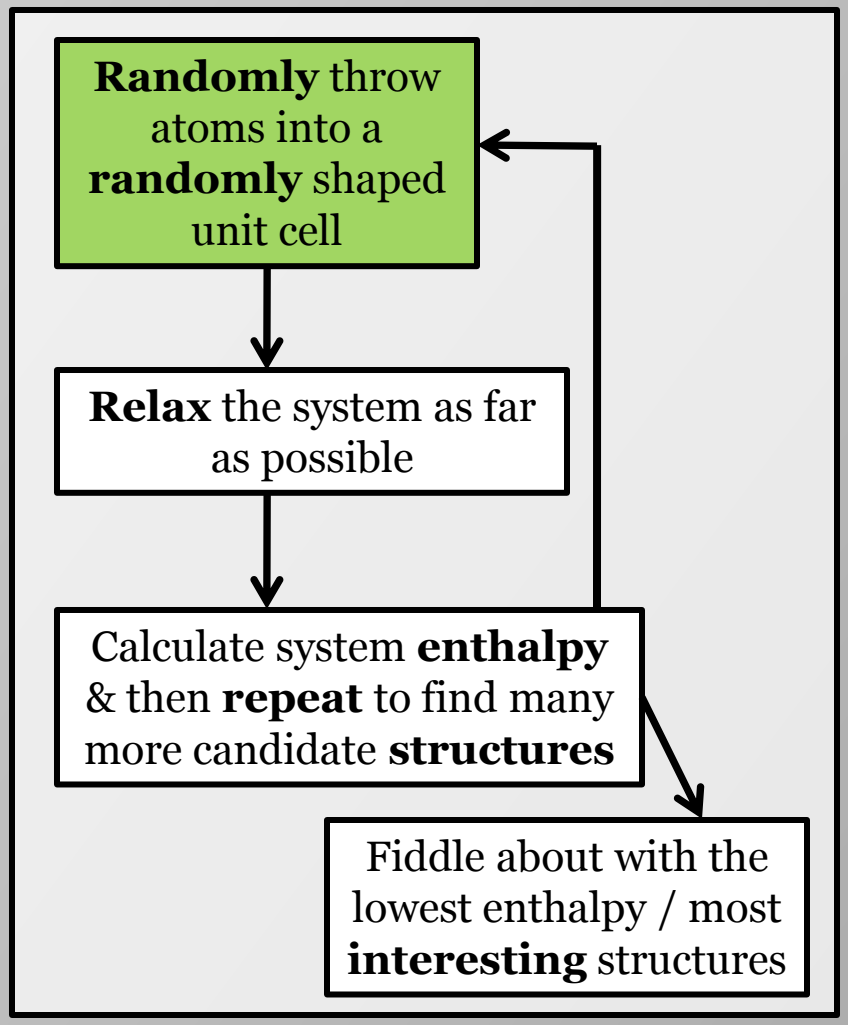
The Problem



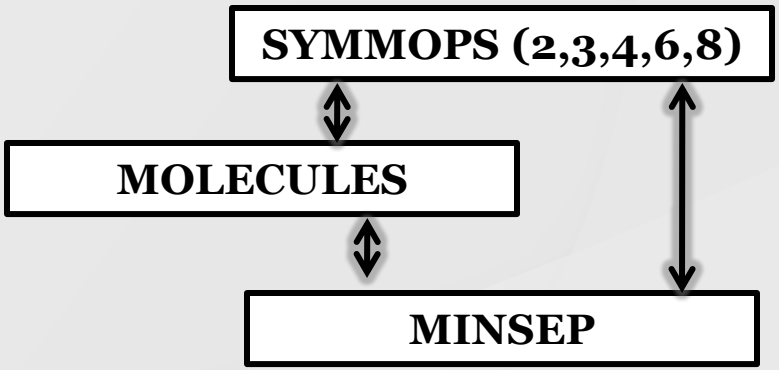


Cotunnite ($PbCl_2$) structure

Random Structure Searching



"One of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition."
J. Maddox *Nature* **335**, 201(1988)



Searching & the Structures

The searches:

~1800 relaxed structures in total

Unconstrained 2 units
Unconstrained 4 units

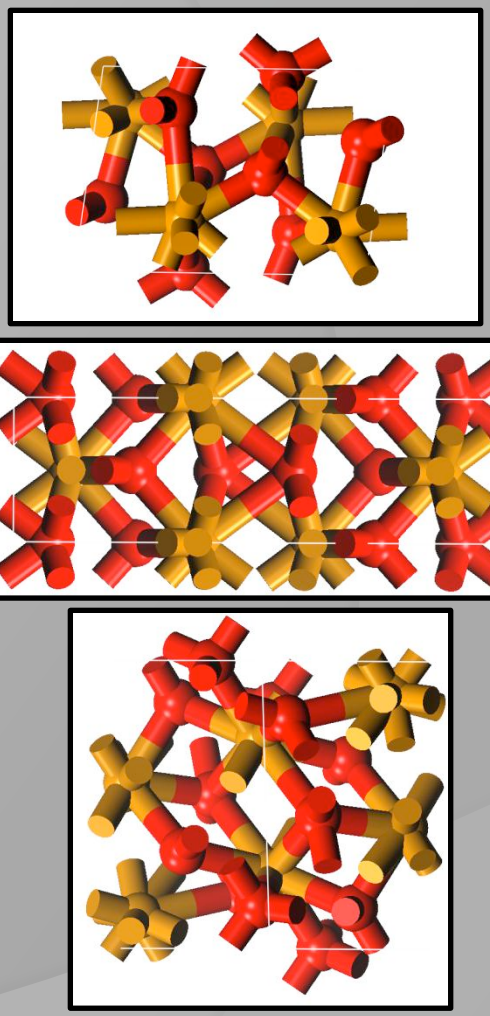
1 unit * 3 symmetry ops.
1 unit * 4 symmetry ops.
1 unit * 6 symmetry ops.
1 unit * 8 symmetry ops.

1 * 120° molecule * 4 symmetry ops.
2 * 120° molecules * 4 symmetry ops.
3 * 120° molecules * 4 symmetry ops.

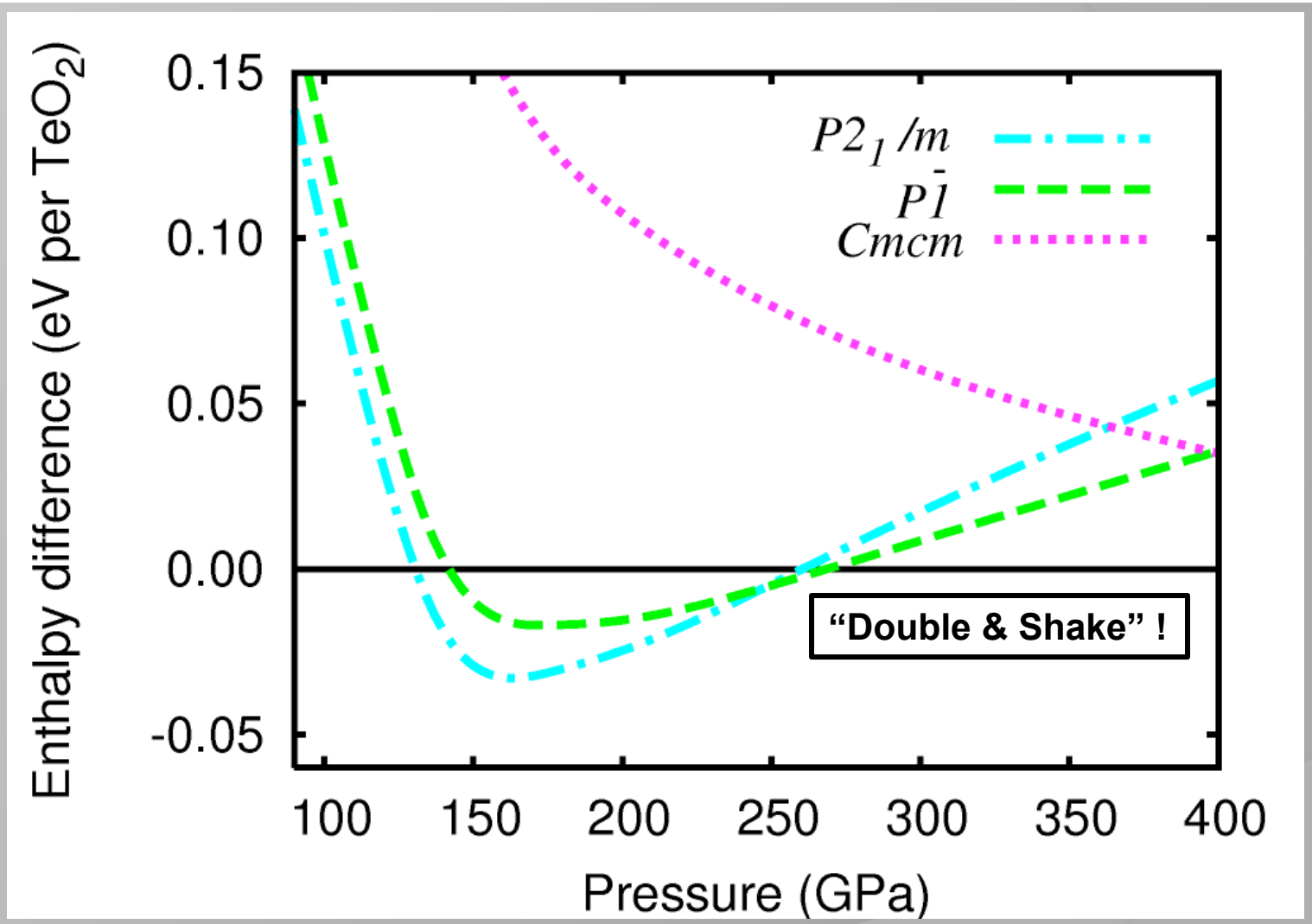
150 GPa

1 * 120° molecule * 4 symmetry ops.
3* 120° molecules * 2 symmetry ops.
4* 120° molecules * 2 symmetry ops.

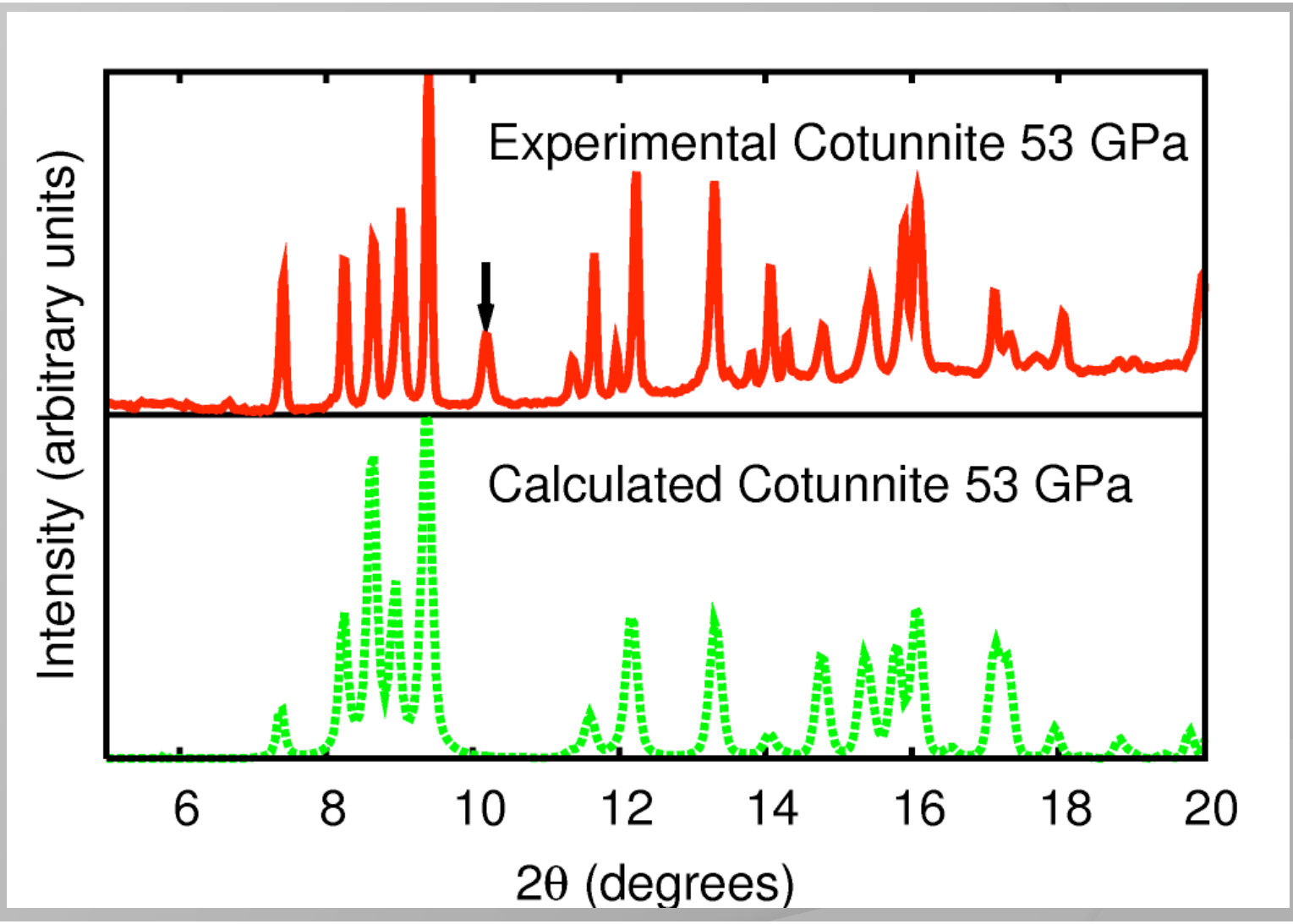
280 GPa



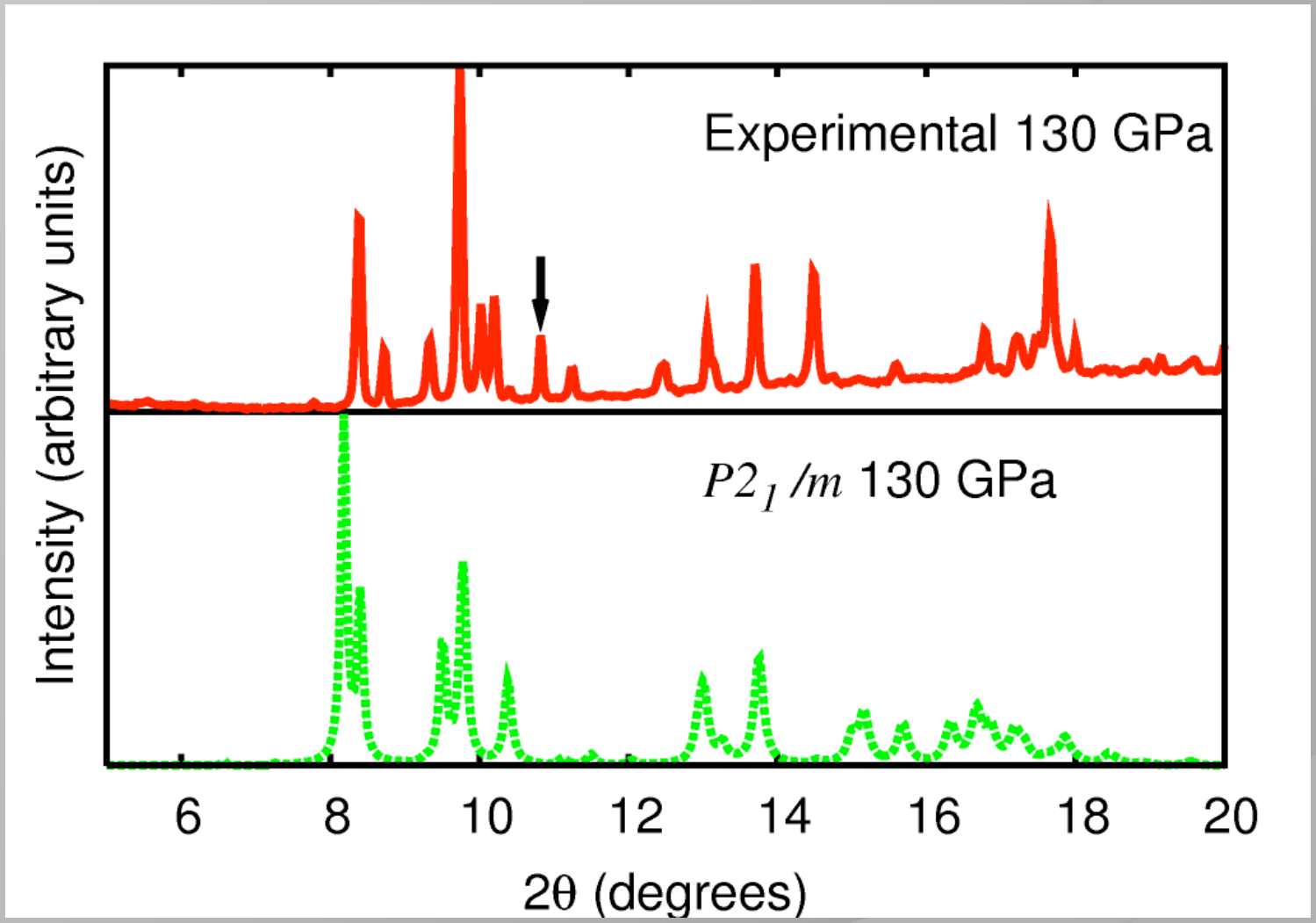
Enthalpy vs Pressure



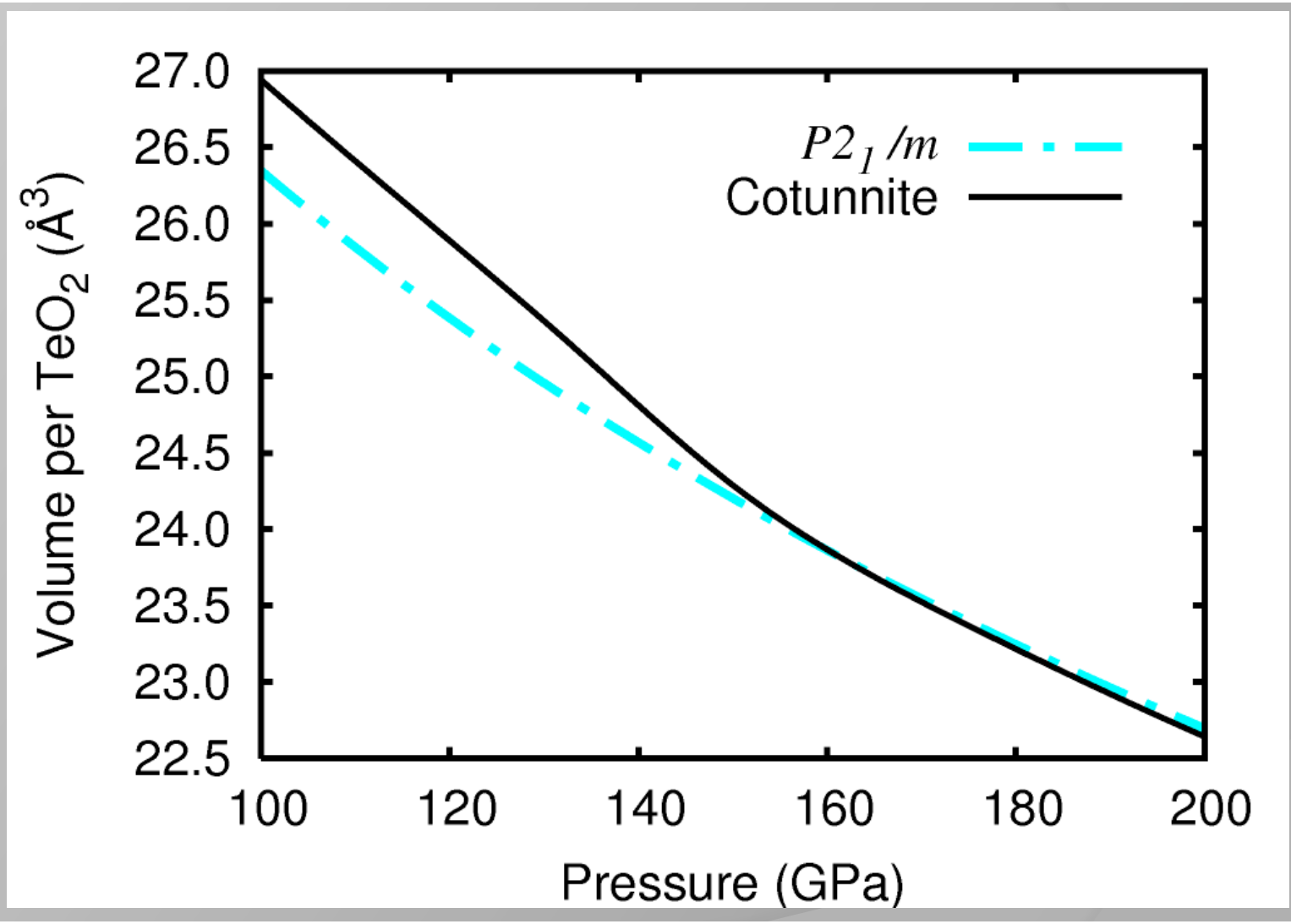
X-ray diffraction



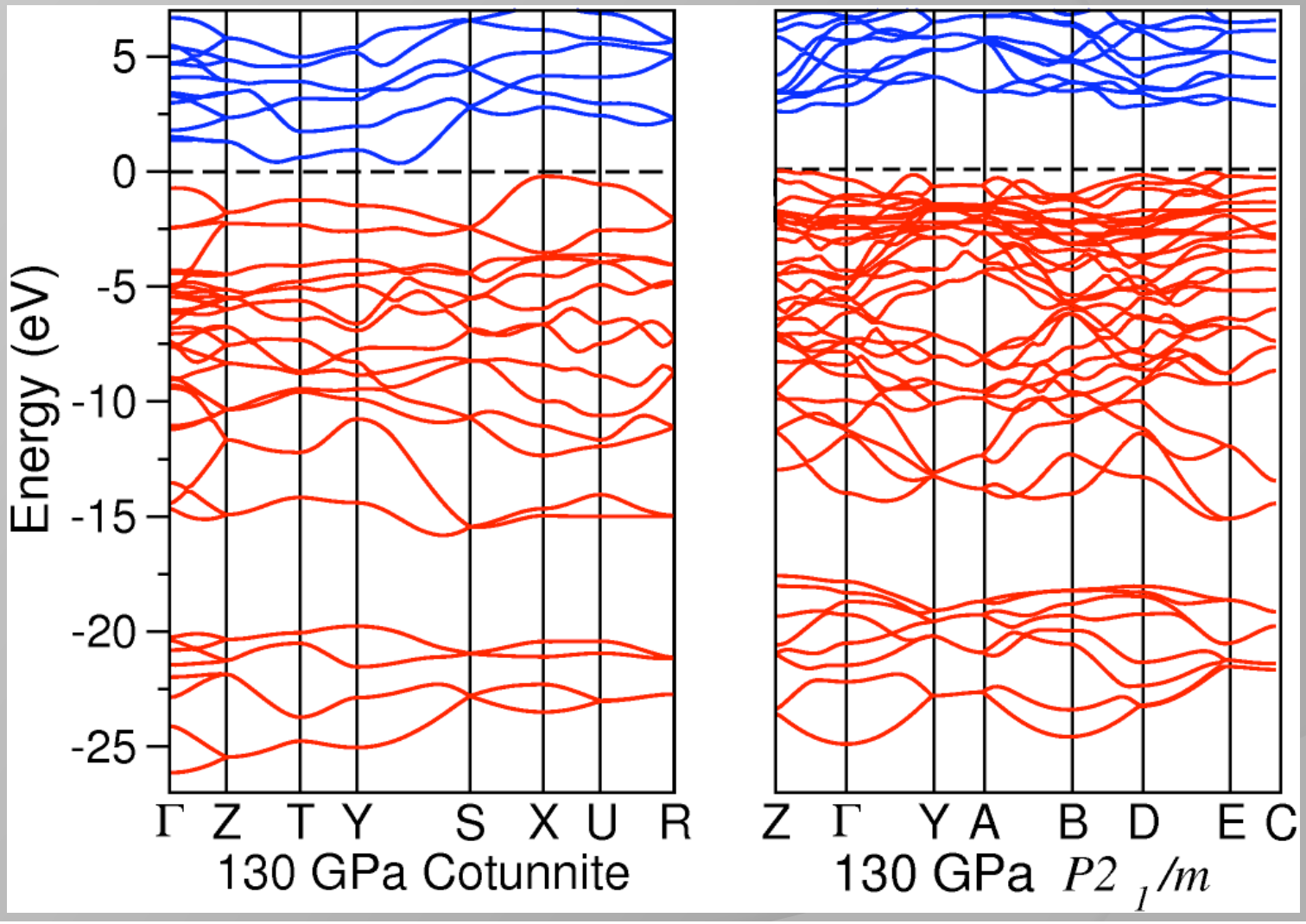
X-ray diffraction



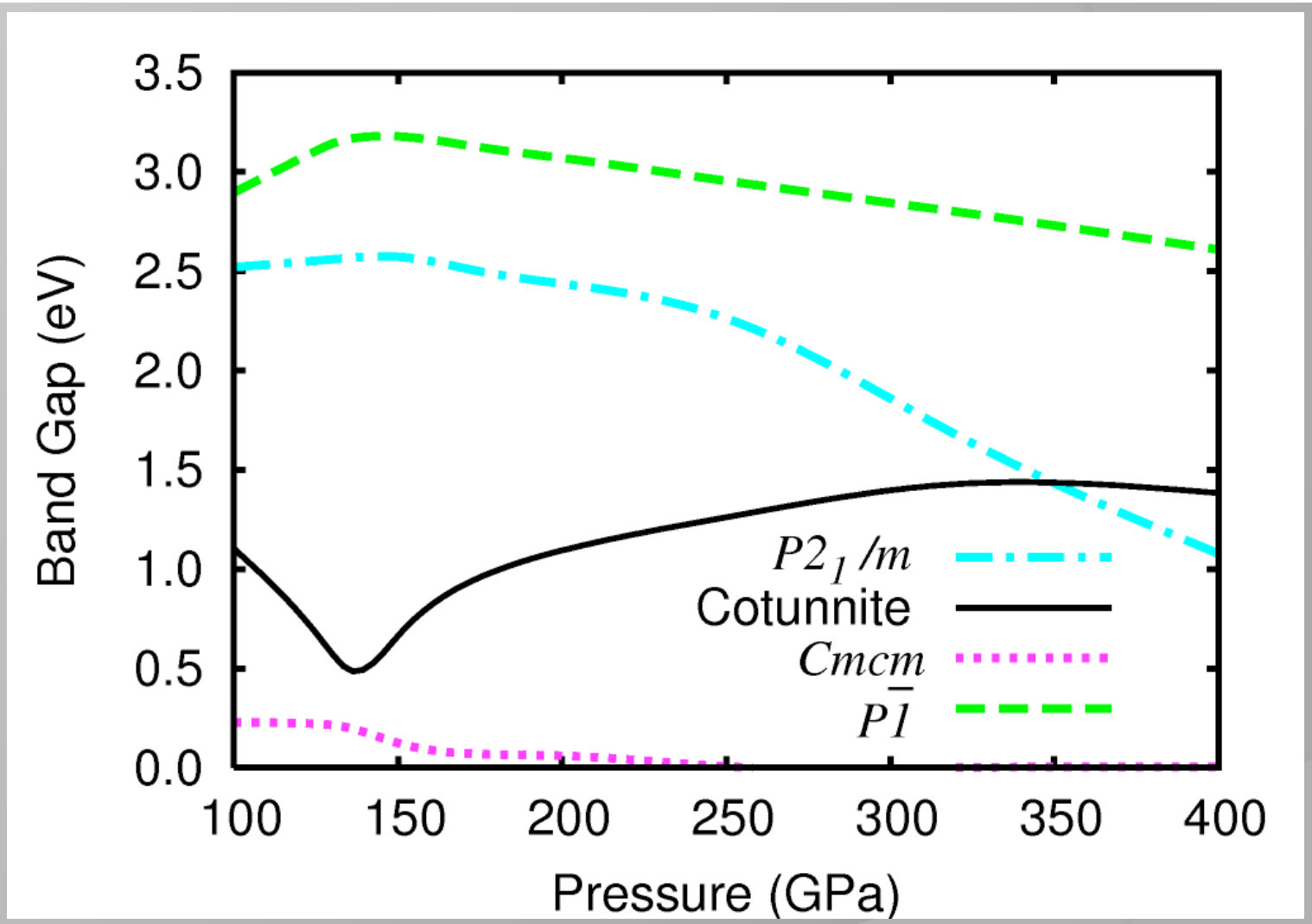
Cotunnite volume 'kink'



Band Structure



Band Gaps


Band Gap (eV)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
100
150
200
250
300
350
400
Pressure (GPa)
$P2_1/m$
Cotunnite
$Cmcm$
$P\bar{1}$

Summary / Conclusions

- Study supports experimental observation of post-cotunnite phase at pressures accessible to a diamond anvil cell.
- Predict transition to *P2$_1$/m* tenfold coordinated phase at 130 Gpa.
- New *P2$_1$/m* phase does not appear to be a general post-cotunnite phase (shame...TiO_2 !)
- Cotunnite re-enters at 260 Gpa
- Higher quality x-ray diffraction data required to confirm.

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Acknowledgments

TCM

EPSRC

Engineering and Physical Sciences Research Council

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