

Project B9



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Lead-free $(100-x)(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3 - x \text{BaTiO}_3$ relaxor ferroelectrics characterized by ^{23}Na Nuclear Magnetic Resonance (NMR)

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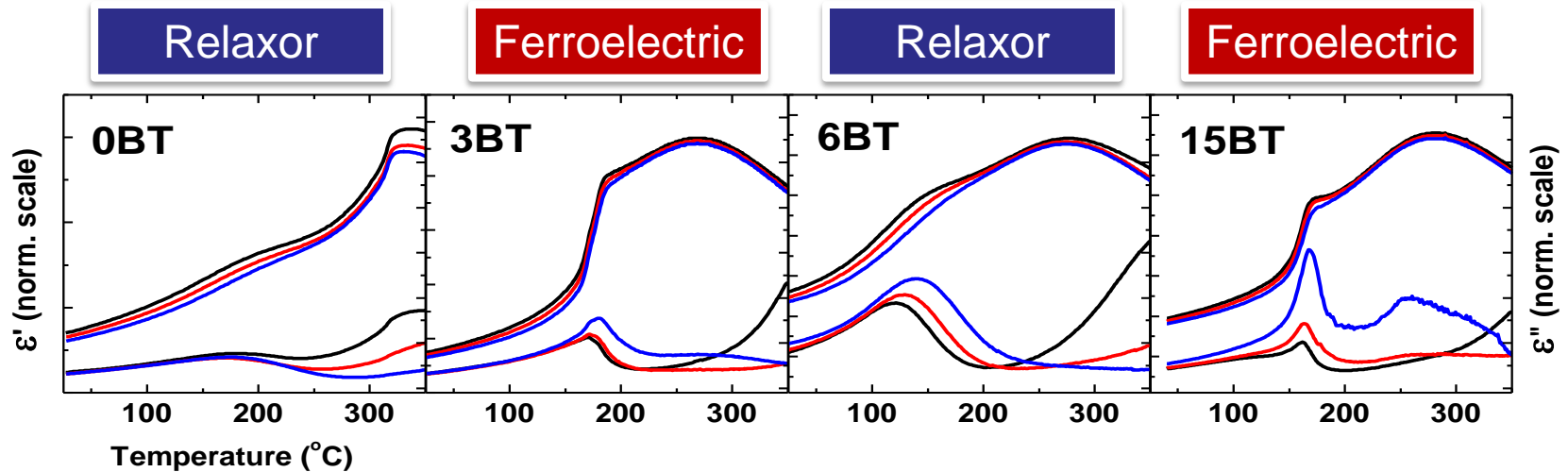
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Germany

² Department of Materials Science, Technische Universität Darmstadt,
Germany

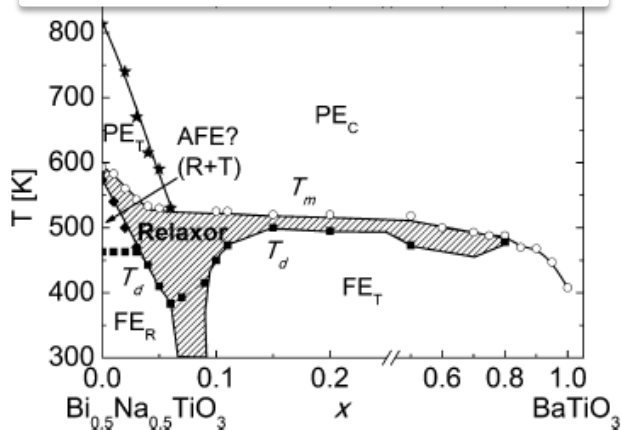
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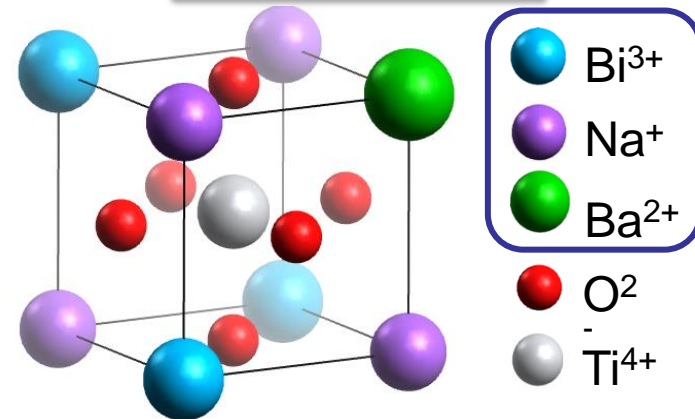
BNT-xBT Relaxor-to-Ferroelectric Crossover



BNT-xBT Phase Diagram



A-Site Disorder



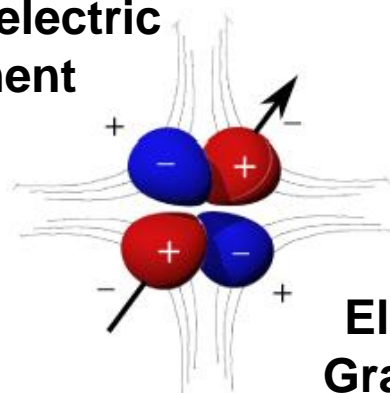


1st Question:

Is there any relation between local structure disorder and the relaxor behavior in BNT-xBT materials?

²³Na Nuclear Magnetic Resonance (NMR) - The Quadrupolar Interaction

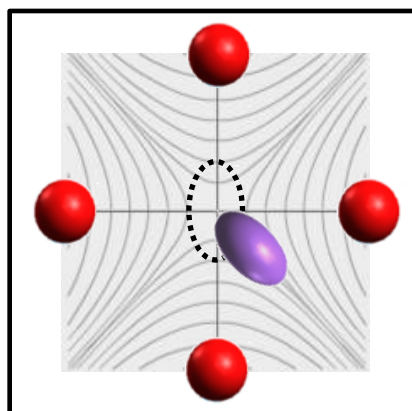
Nuclear electric
moment



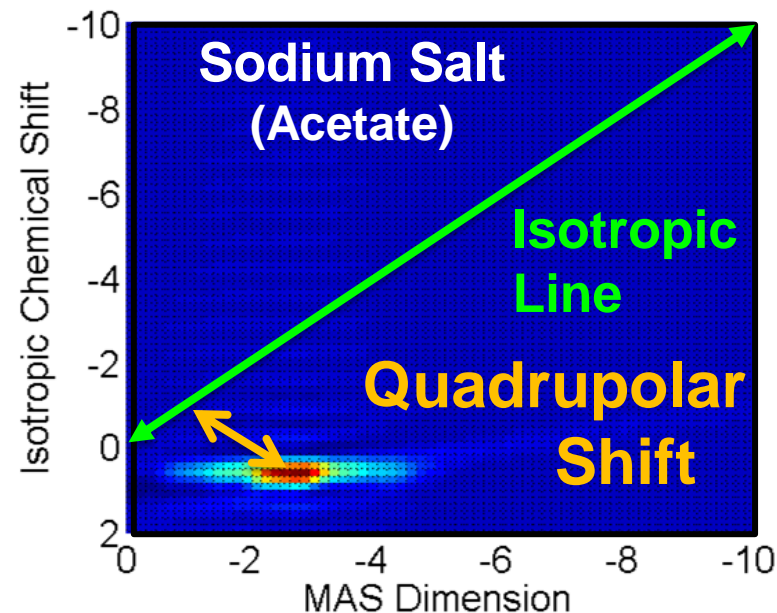
Electric Field
Gradient (EFG)

EFG \propto

- r^{-3}
- **Distortion**

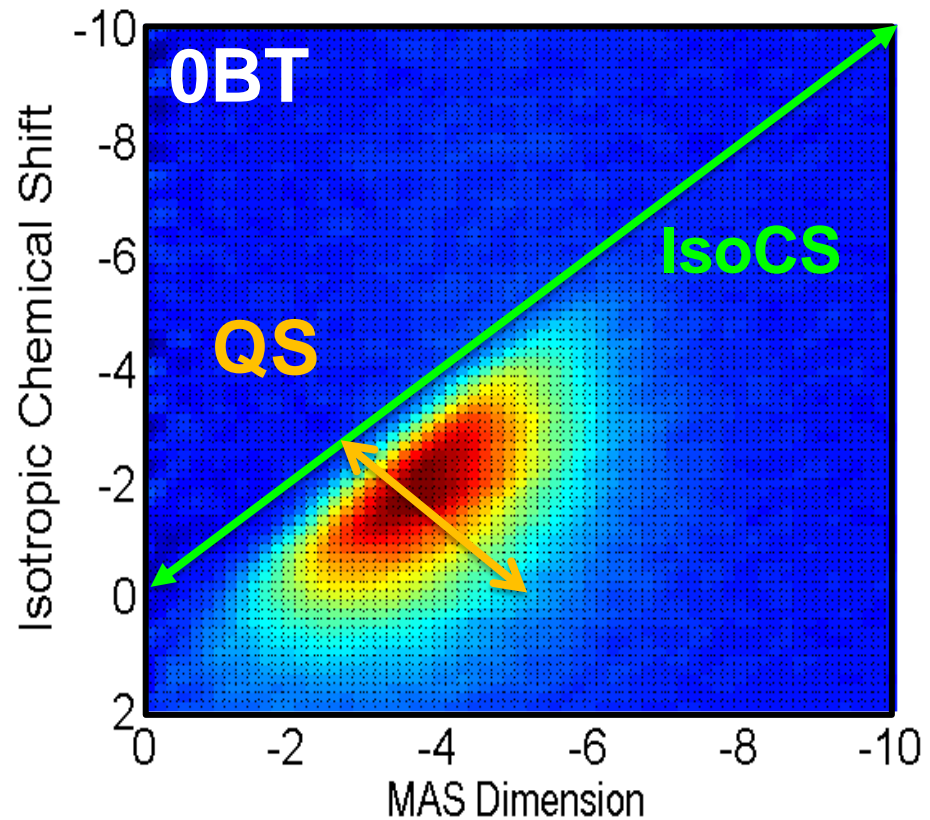
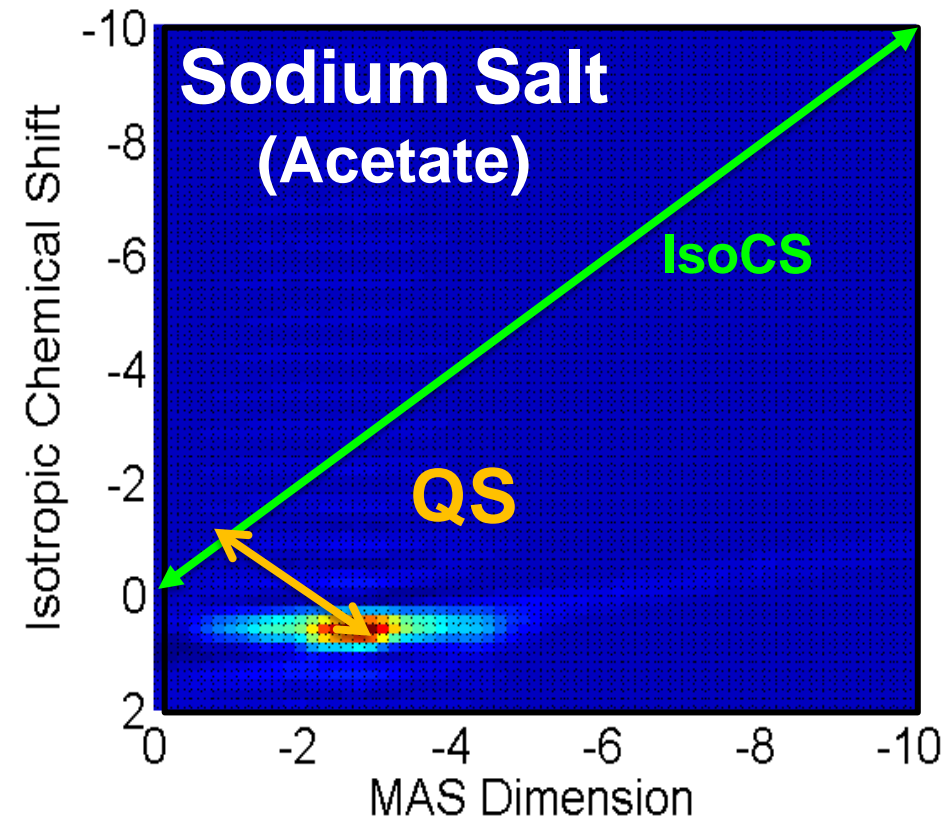


²³Na 3QMAS NMR

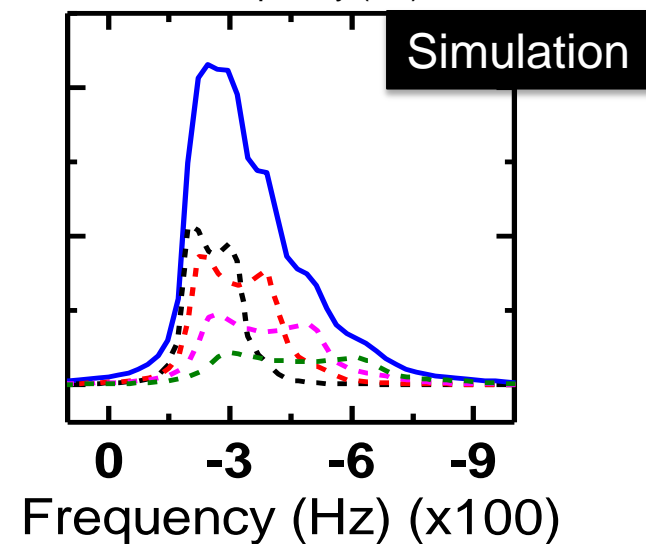
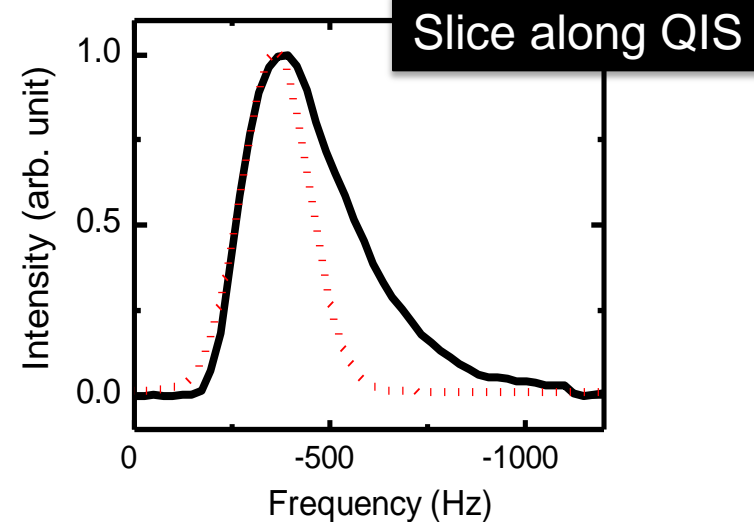
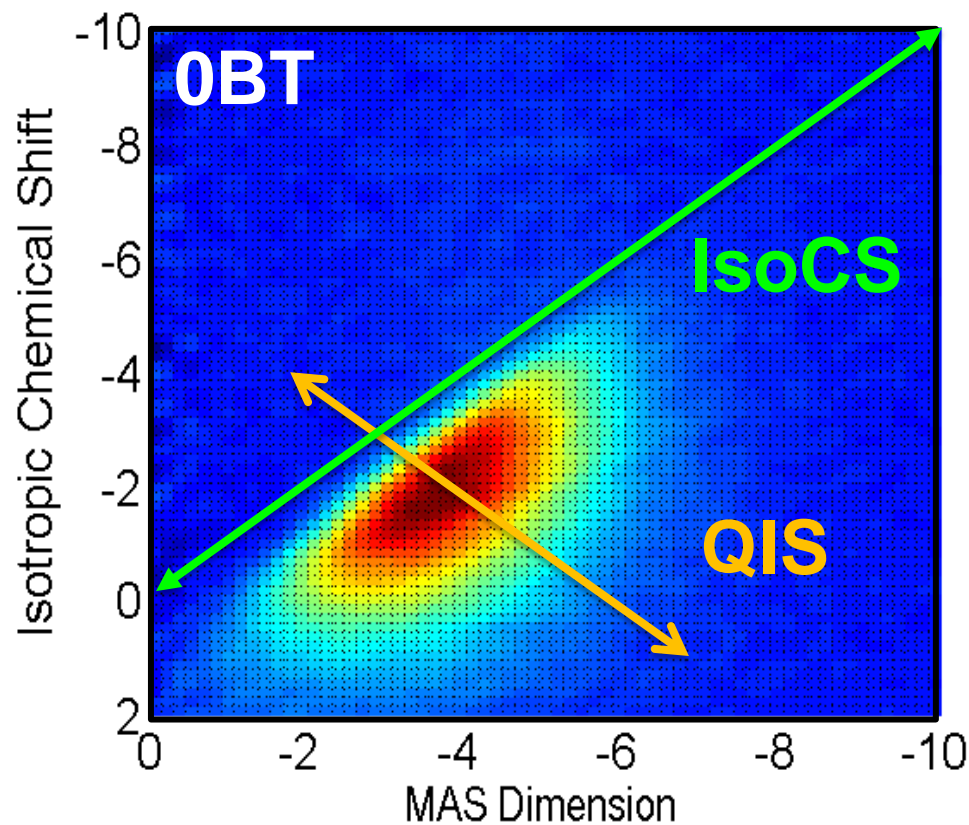


- High resolution
- Quadrupolar Shift
– measure of distortion
- Ordered material - ridge

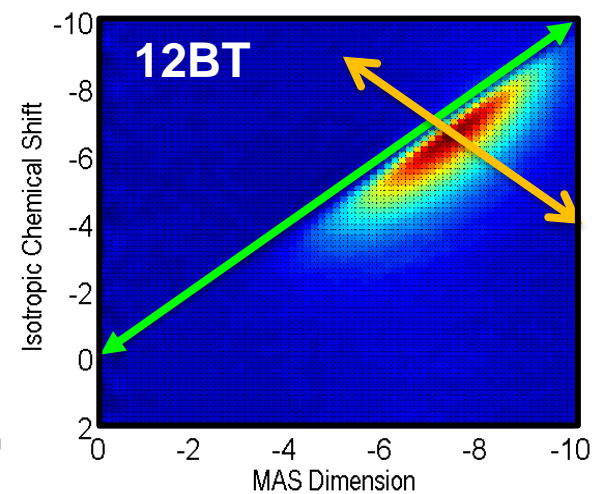
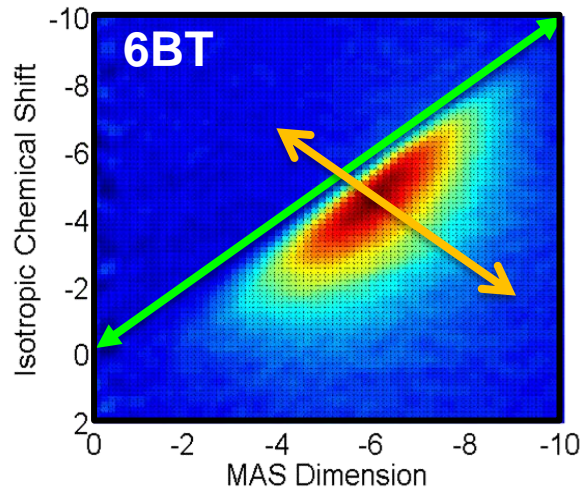
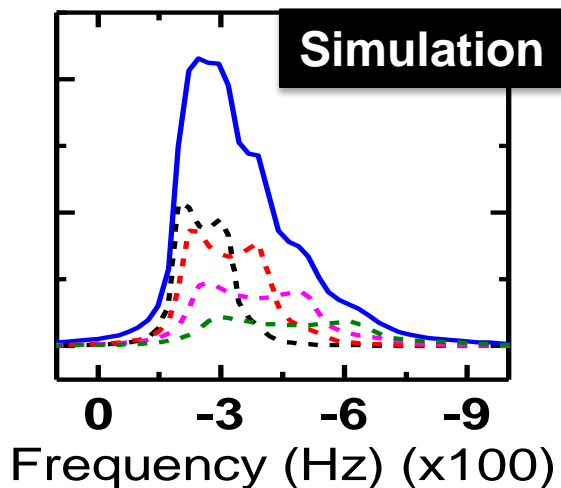
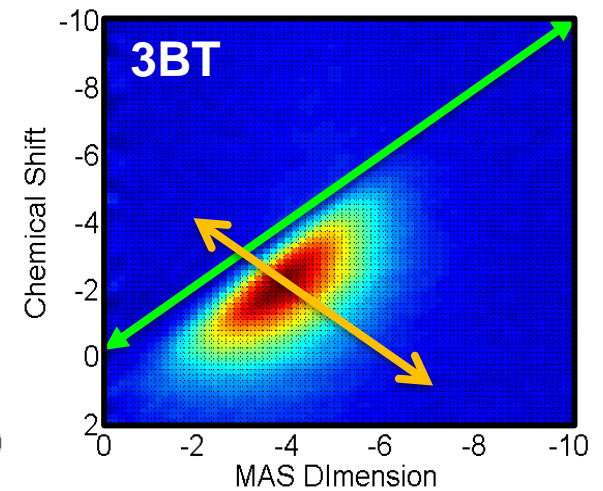
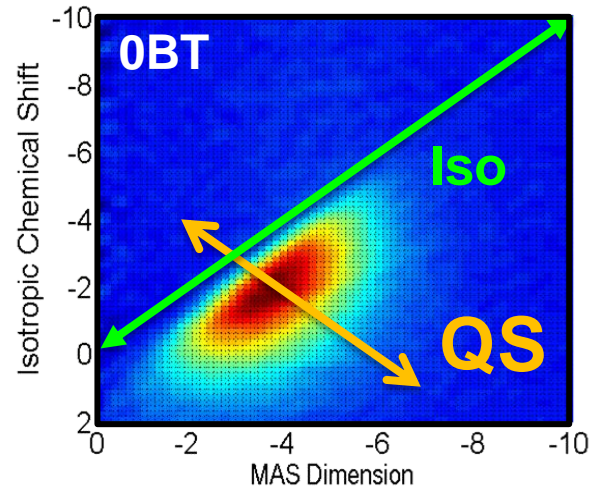
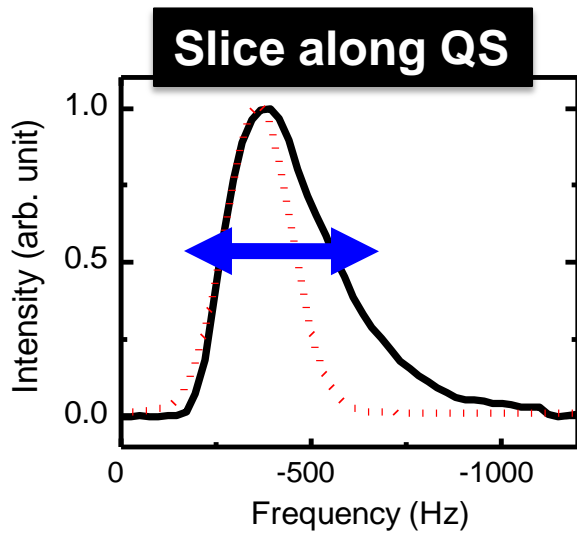
3QMAS – pure BNT – Local scale disorder



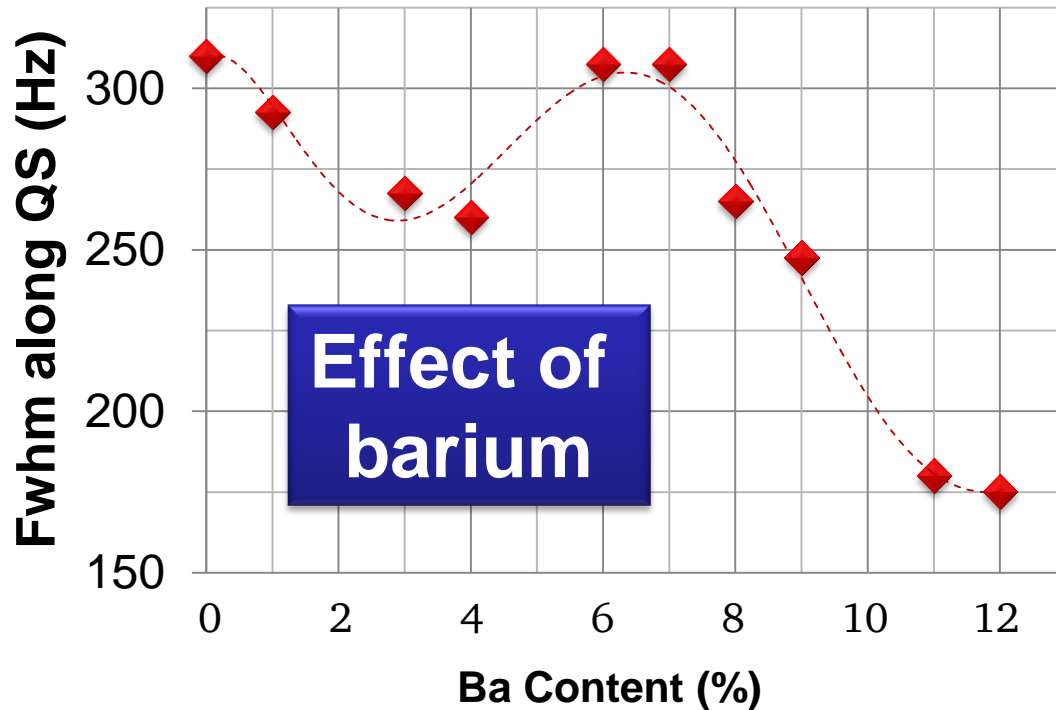
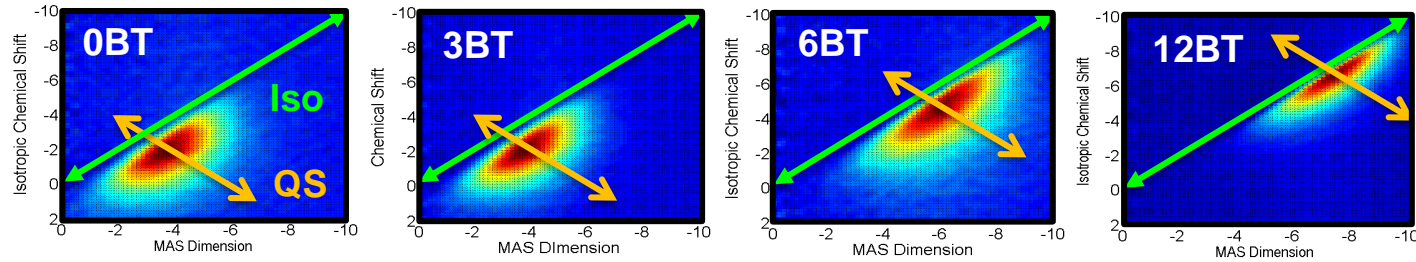
3QMAS – Distribution of Quadrupolar Interaction



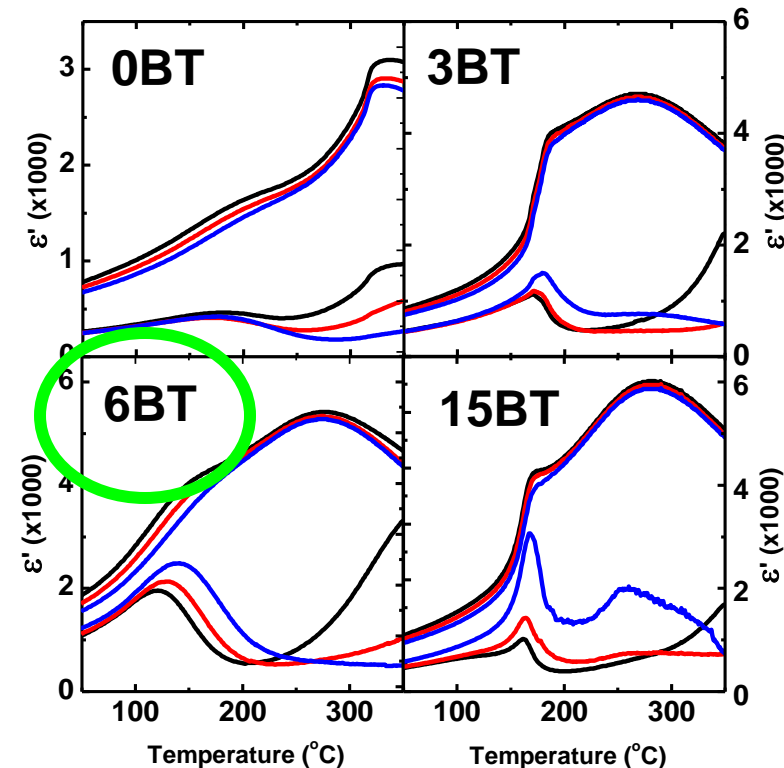
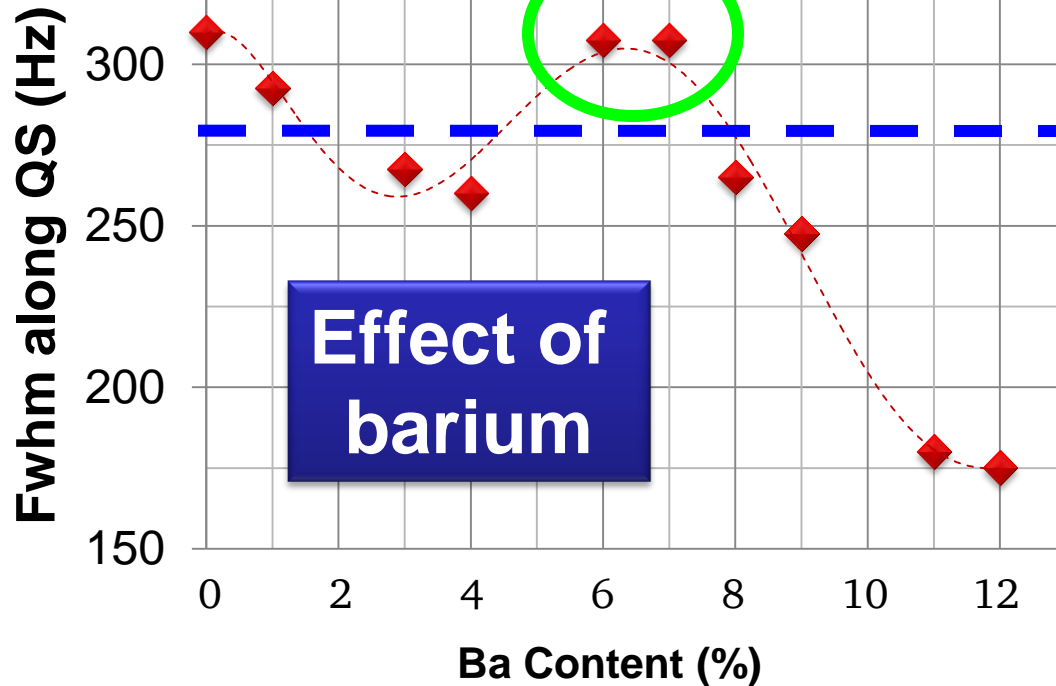
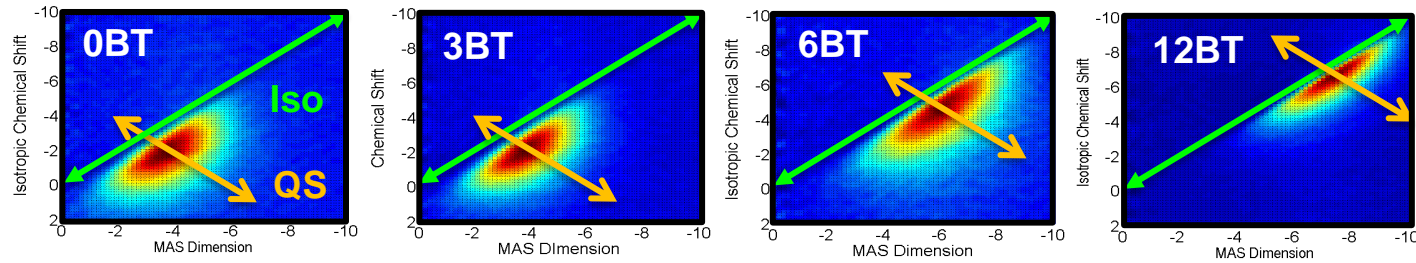
3QMAS – Quadrupolar Interaction Only!



Local disorder dependence to xBT content contrasted to the permittivity



Local disorder dependence to xBT content contrasted to the permittivity

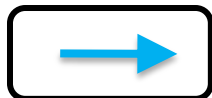
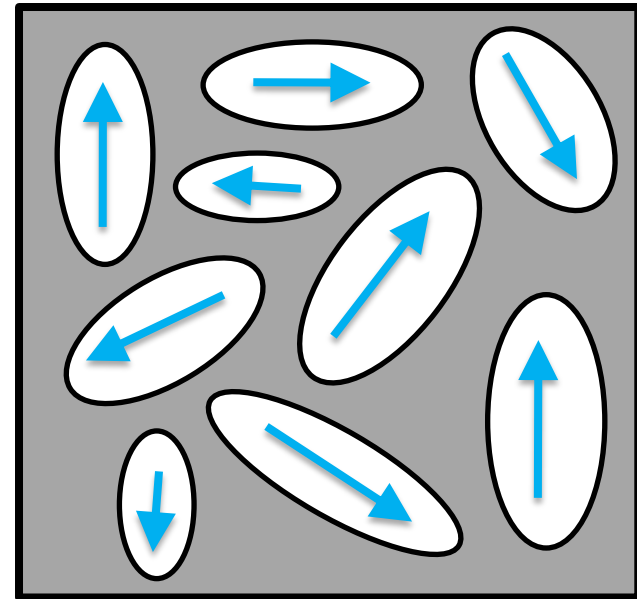
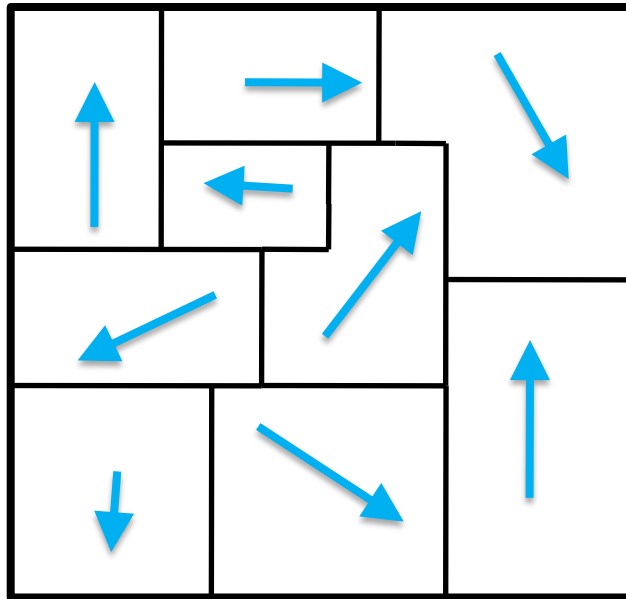




2nd Question:

What other effects can account for relaxor behavior in BNT-6BT?

BNT-6BT & Nano scale structure of Relaxor Ferroelectrics



Local Polarization

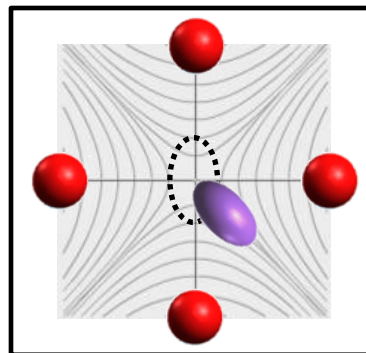
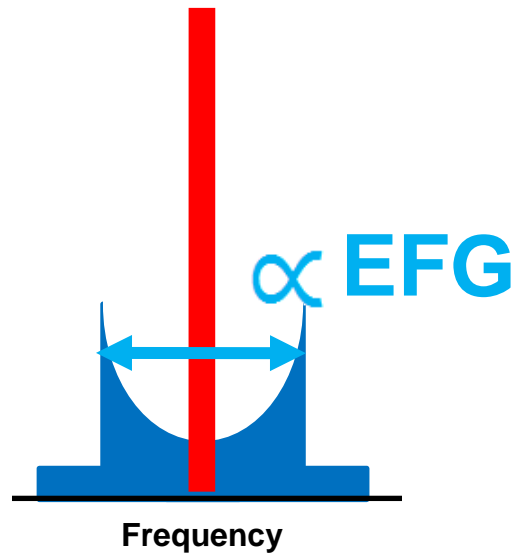


Non-polar
Matrix

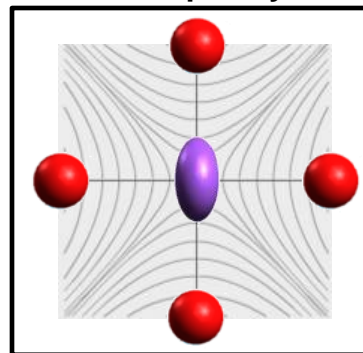
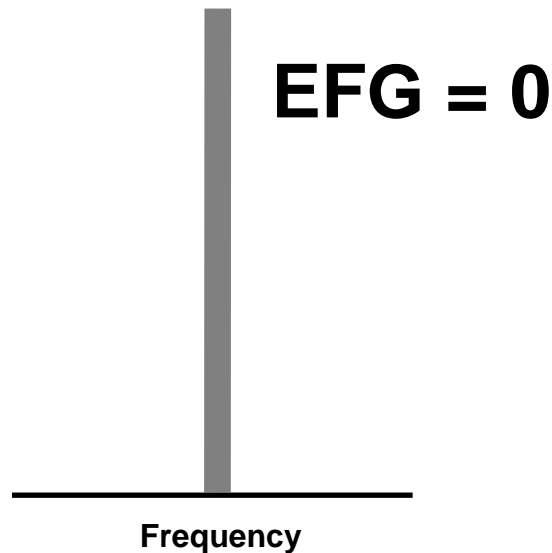
Adapted from: Bokov, A. A; Ye, Z. G., J Mater Sci **41**, 31 (2006)

^{23}Na ($I=3/2$) NMR – 1st Order Quadrupole Interaction

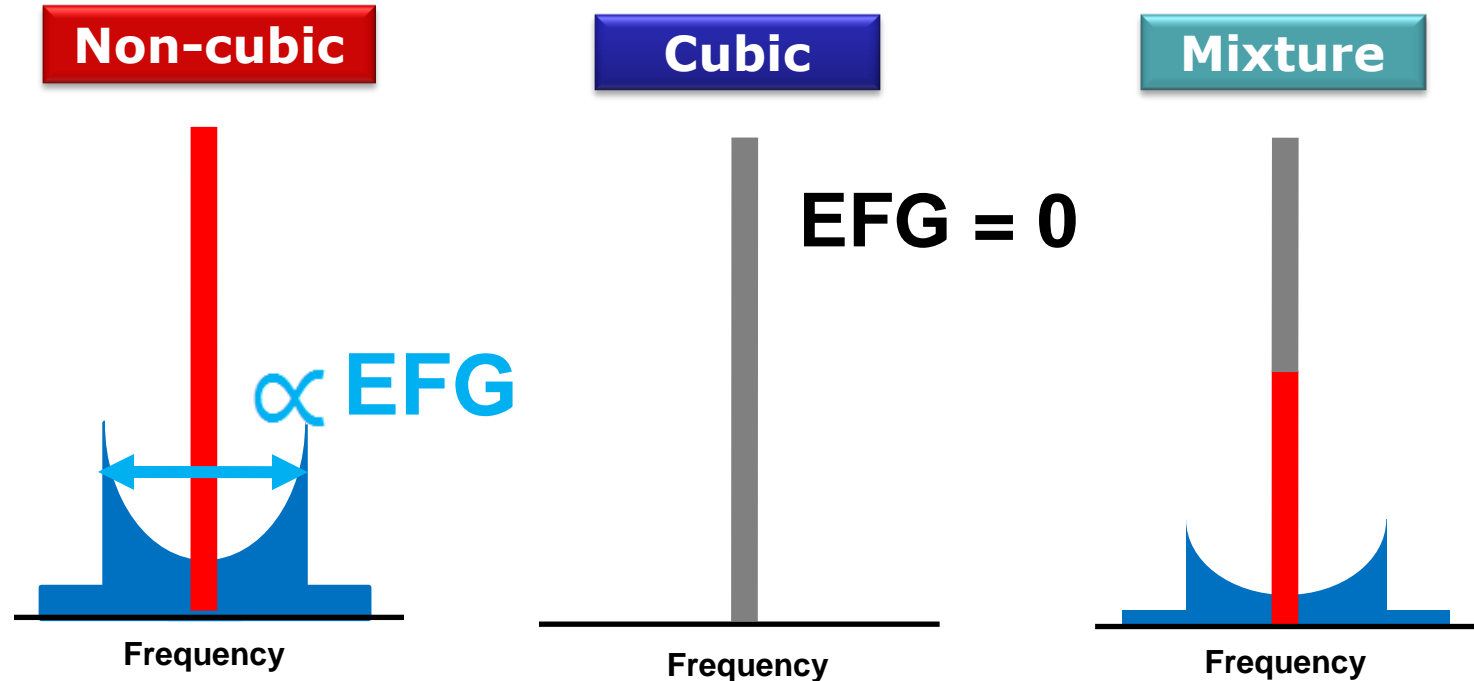
Non-cubic



Cubic



^{23}Na ($I=3/2$) NMR – 1st Order Quadrupole Interaction

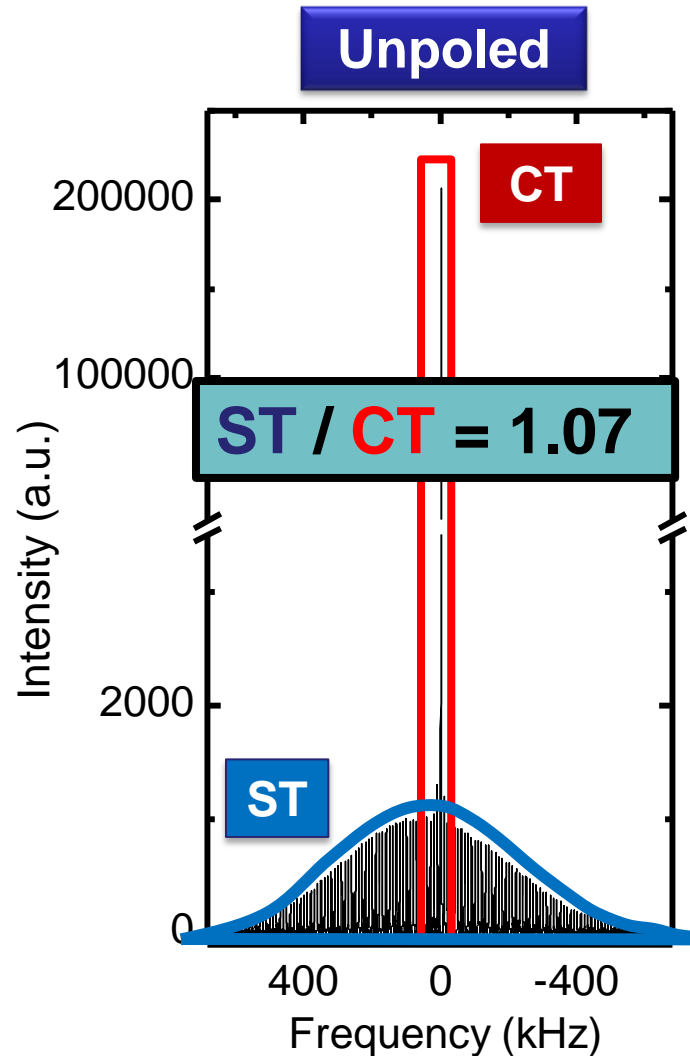


$$\frac{\text{ST}}{\text{CT}} = 1.5$$

$$\text{Overall Ratio} < 1.5$$

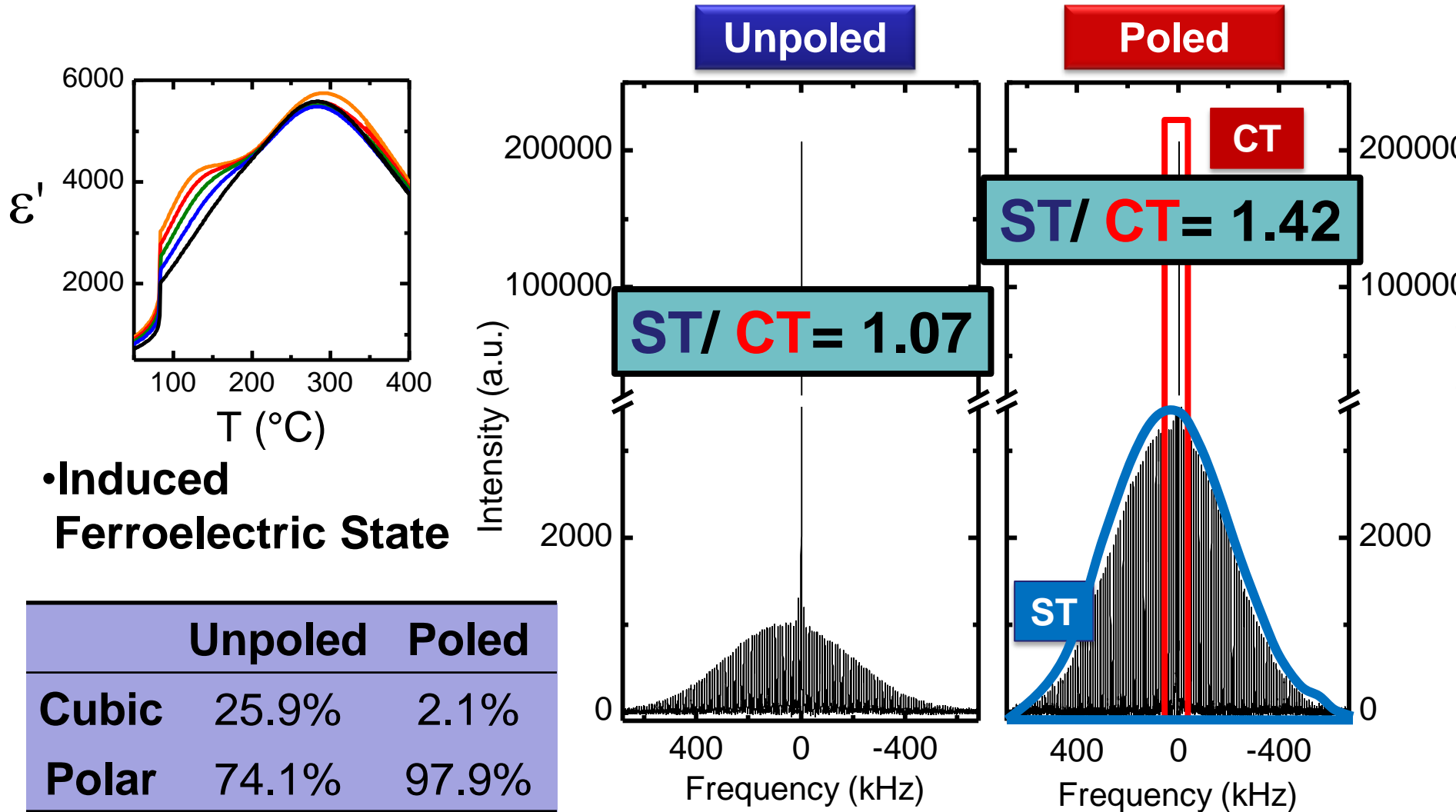
^{23}Na MAS NMR of *unpoled* BNT-6BT

- **Relaxor State**
 - Cubic to XRD
- **Polar** (non-cubic) symmetry
 - Nanometric character
- **Distribution of EFGs**
 - Partial Disorder

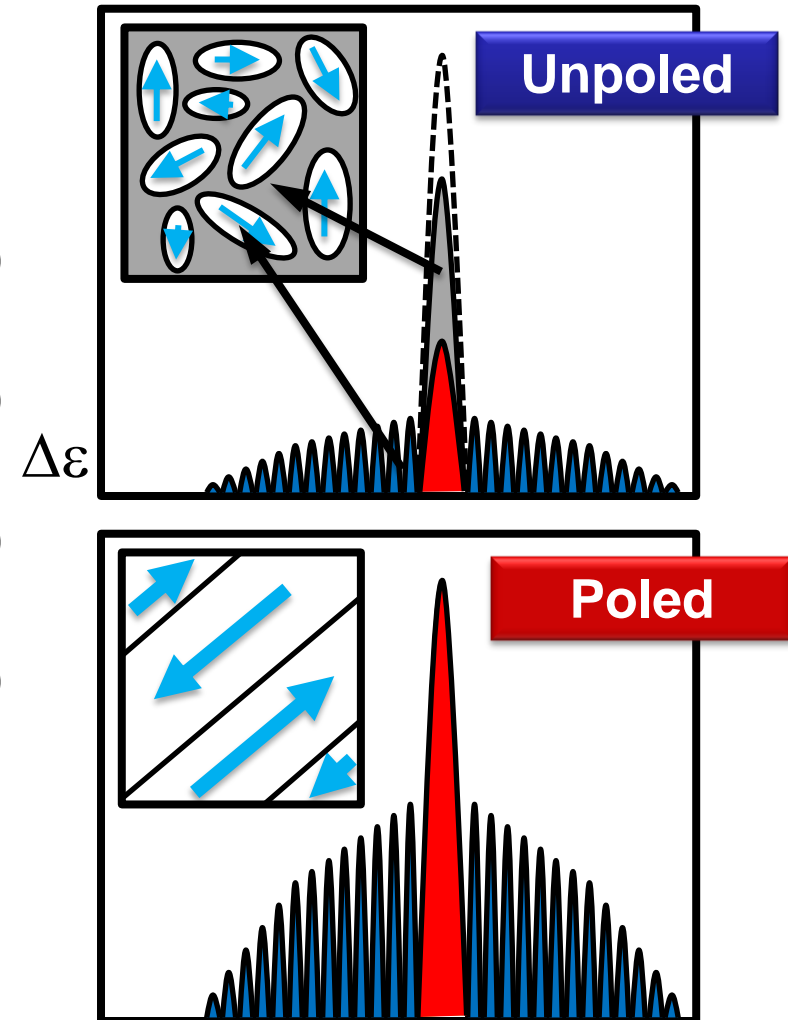
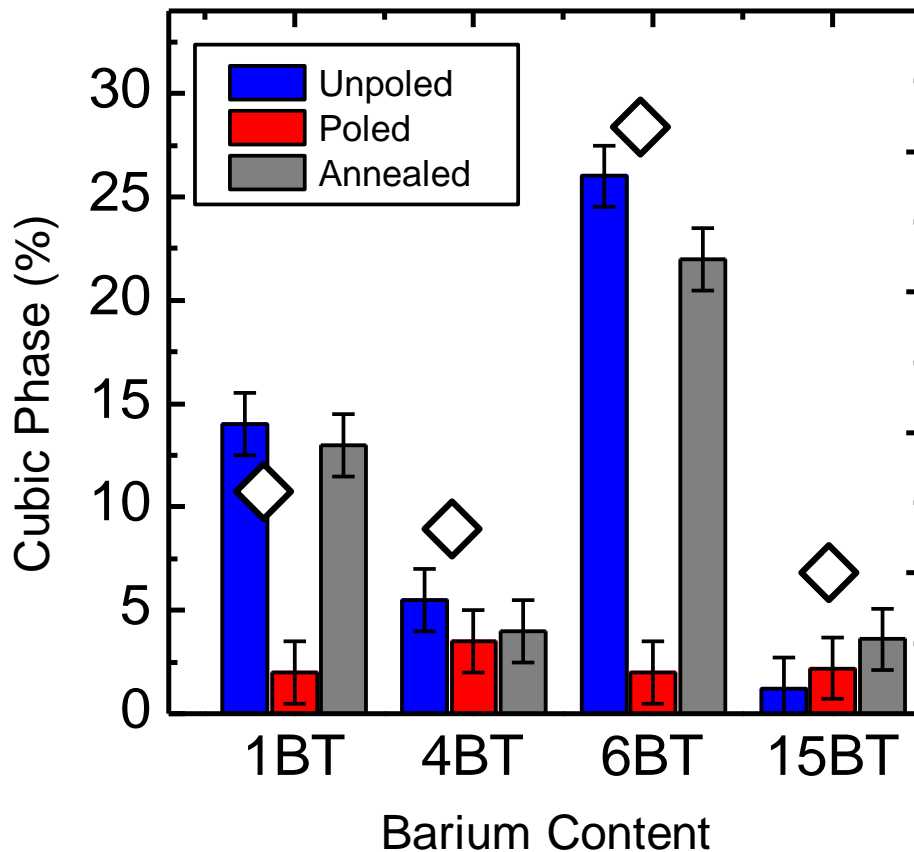


- **Two Phases**
 - $74.1\% \pm 2.0\%$ **PNRs**
 - $25.9\% \pm 2.0\%$ **Cubic**

^{23}Na MAS NMR of *poled* BNT-6BT



Cubic/non-cubic Phase Coexistence



Conclusions

- ^{23}Na NMR sensitive the local structure and the degree of disorder in BNT-xBT materials;

Acknowledgements

Prof. Buntkowsky's Group
Dr. Hergen Breitzke

Prof. Rödel's Group



Thank you for your attention!