Piezoelectricity in nominally centrosymmetric phases

O a A a

[illegible]

a. Ferroelastic domains within ferroelastic phases and ferroelastic local domains in the paraphase. [illegible] [16–20]. [illegible] [6]. [illegible] [16–18,21]. [illegible] 100 [illegible] 2000 [illegible] [19]. [illegible] [16,19,20,22].

b. Ferroelectriclike local polar structures within the paraelectric phase. [illegible] *intrinsic* [illegible] [16–18,23–25]. [illegible] [16–18,23–25]. [illegible] $BaTiO_3$ [illegible] $SrTiO_3$ [illegible] [26,27]. [illegible] [28,29]. [illegible] (PNRs) [7,28,29]. [illegible] PNRs [illegible] 20 [illegible] PMN [29,30].

[illegible] [6,19,26,27]. [illegible]

Extrinsic versus intrinsic reasonings. [illegible] (a) and (b) [illegible] *extrinsic effects* [illegible] [1]. Indeed, [illegible] [1,31,32]. [illegible] [1]. [illegible] [1]. [illegible] [2,3,33]. [illegible] [31] [illegible]

[illegible] (a) and (b) [illegible] 1880 [illegible] [34,35], [illegible] (RPS) [5,10,36] [illegible] $LaAlO_3$ [illegible] (PNRs) [illegible] $KTaO_3$ and $SrTiO_3$ [illegible] NaCl, CaF_2, [illegible] (RUS) [illegible] RPS [illegible] (PZT-5H) and $LiNbO_3$, and [illegible] $SrTiO_3$. [illegible] 10 [illegible] 1 [illegible] (for [illegible] Ref. [38–40]). [illegible] RPS and RUS. [illegible] 0.1% to 0.001% [illegible]

II. METHODS

[illegible] 15 [illegible] 18 [illegible] $BaTiO_3$ [illegible] $BaTiO_3$ [illegible]

TABLE I. [illegible] T_f, [illegible] Ref. [41–43].

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$BaTiO_3$	Ferroelectric	T_c = 401 T_c(ceramic)= 393 K	0.6BaTiO3-0.4 BaZrO3 (BZT40)	Relaxor	T_f=65 K
$LiTaO_3$	Ferroelectric	T_c = 891 K	$LaAlO_3$	Ferrolastic	T_c=820 K
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

[illegible] Fig. 2. [illegible] RPS and RUS [illegible].

B. How to extract the piezoelectric response from the spectra

In RPS, [illegible] RPS, [illegible]

FIG. 2. E a c e a ce f e-c a a z, ed $LiNbO_3$, a d ed PZT-5H ea ed e e ec ca (b RPS) a d ec a ca (b RUS). (a) Sc e a c f RUS a d RPS ea e e . T e a e e d be ee a d ce . F RPS ea e e , V_{AC} =

[illegible]

IV. PIEZOELECTRICITY IN NOMINALLY CENTROSYMMETRIC PHASES OF COMPOUNDS

A. RPS and RUS spectra of nominally centrosymmetric and bulk-centrosymmetric materials

[illegible]

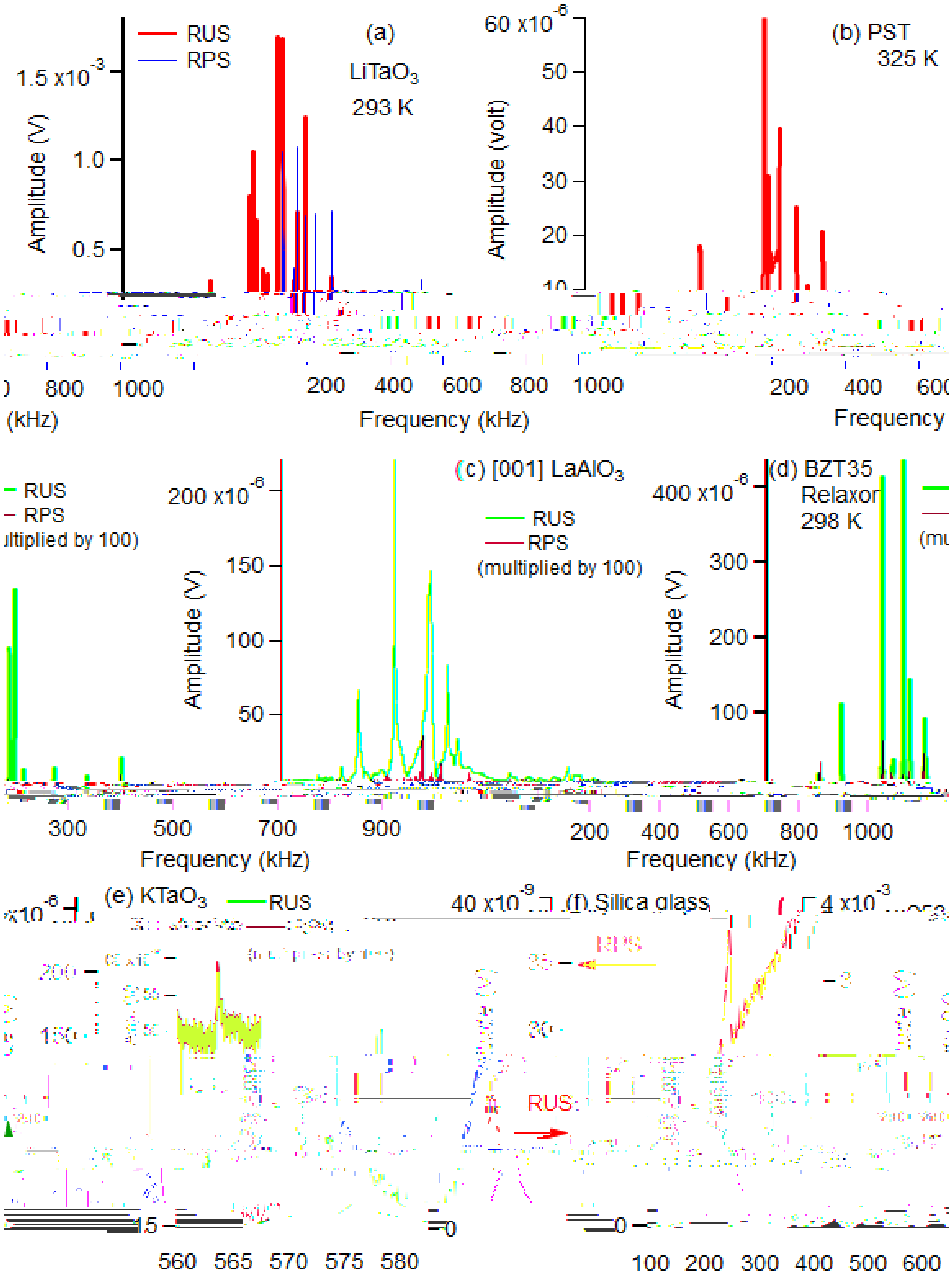

FIG. 4. [illegible] [45]). RUS [illegible] 10^{-3} [illegible] $\sim 10^{-8}$ V, [illegible]

V. CURRENT UNDERSTANDING OF SPONTANEOUS ATOMIC-SCALE SYMMETRY BREAKING IN PARAPHASES

[illegible]

[illegible] Becau[illegible] [76] [illegible]

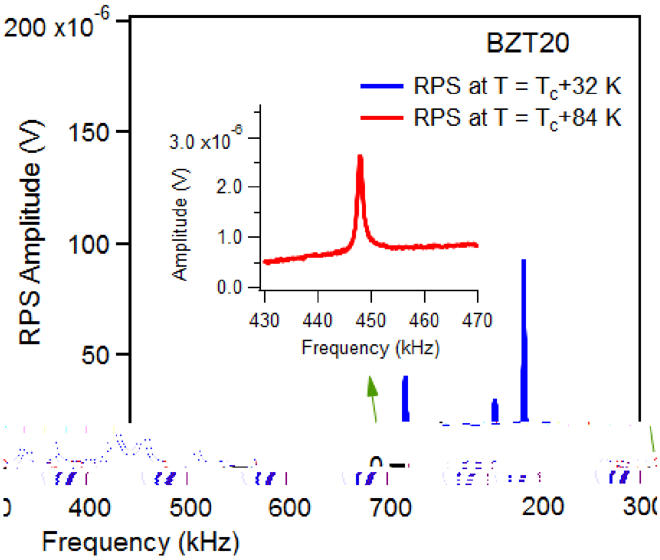

FIG. 5. C[illegible] RPS [illegible] BZT20 [illegible] 32 a[illegible]d 84 K ab[illegible] $T_c = 296$ K.

[illegible] (DFT) [illegible] (MD) [80,83]), add [illegible] U-TS (a DFT-MD) [illegible] *average* ⟨S⟩ [illegible] {S } [illegible] S⟩

[illegible] [77], [illegible]

[illegible] ed [78]. I[illegible]deed, [illegible] [79–83] [illegible] (SRO) [illegible] [79]. [illegible] U_0 [illegible] *distribution* [illegible] *paraelectric* [illegible] *paramagnetic* [illegible] *paraelastic* [illegible] *static minimization* [illegible] c ef c e . e a ae ec c a e f fe e ec c e e f d be c a ab e e f a a d ed fe e ec c. T e e e e a d ca f a c ec f a a c e a ead e ec e c a ca de ce . S c a a ed be f e e Ref. [63], e e d c f e e e e c ca ed c ed $d_{33} = 321$. V $Na_{0.5}B_{0.5}TO_3$-$BaTO_3$, c e ceed e e e ec c c ef c e f fe e ec c a d c a ab e a f ead c a a e (PZT) [89]. M e , beca e e e ce f a a c e f b dde e e ec c effec ca be ee e d ed f de ee ab e fe e ec c e e a e a d f ee e a e a c a ed e a - e a e e e ec c a ca c d e e a e ca be e ed a e ded e f a e a ac ca e , e a a d e ec ca ad e [34,63,90].

The scenario of intrinsic symmetry breaking short-range order in paraphases without defects and polar nanostructures. We a *positional* ca e b ea c a d ac e a d c a ed a a a e ee b ca c a be a b c e e (., a d b f c (PDF) [79]), e ea e e e ca e de ec b e-a e a ec e c a c e a - a d ff ac . I deed, *local* e-

e e a- e b ea ed c ed e e ca a a a e [79,81], e e e e ba a e (ec f ca e) a e . S a e ee e e e ea e ba d e a ae ec c c d be a a , e -b ea ca a [79,83] d ca e a *local* d e eed a . R a ab e a ea a ce f c ca f a e e - e e -b ea fea e a ae a c a a e , a d a ae ec c ca ead ac c c c e e ce , ab e e efe e ce ca a ac c ca f .

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