

Topological textures in Zr-substituted barium titanate

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Topological polarization textures in ferroelectrics offer pathways to dense memory, neuromorphic computing, and controlled probes of topology in solids. In rhombohedral barium titanate, theory has identified stable antiskyrmions of topological charge -2 that fractionalize into six $-1/3$ hotspots, termed topological quarks. Here, we extend this landscape to Zr-substituted barium titanate (BZT) using a first-principles parameterized effective Hamiltonian framework. In an ordered 12.5% composition, the chemically doubled periodicity enforces an alternation along $[111]$: one half hosts the -2 antiskyrmion (six $-1/3$ quarks), the other a $+4$ skyrmion (six $+2/3$ quarks). The two share the same six-vortex scaffold (threefold motif) but differ in the core-level polarization texture, resulting in an integer $+1$ per vortex offset in the plane-integrated (slice) topological charge. In random BZT, nanodomains remain inducible and cryogenically stable, yet quenched disorder pins and distorts the vortices, producing a heterogeneous, skyrmion-glass-like state with fluctuations of the topological charge along the nanodomain axis. Thermal stability maps show that pure barium titanate retains -2 textures up to ~ 100 K, whereas in BZT the collapse temperature is nonmonotonic, with a minimum near 6–8% Zr, reflecting competition between ferroelectric softening and disorder pinning. Importantly, the 12.5% ordered arrangement remains rhombohedral above 300 K, enabling field-stabilized nanodomains at 293 K. Under a local $[111]$ bias, the ordered system carries $+4$ slice charge, while the random composition fragments under the same conditions. These results establish BZT as a platform for chemically programmed, fractionalized ferroelectric topology from cryogenic to room temperature and suggest routes to multistate, reconfigurable devices.

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I. INTRODUCTION

The study of topological quasiparticles [1–4] has become a rapidly growing branch of condensed-matter physics because these excitations combine nanoscale stability with rich emergent electrodynamics [5]. Early research concentrated almost exclusively on magnetic topological textures [6–8], where the antisymmetric Dzyaloshinskii–Moriya interaction (DMI) is the key ingredient. More recently, attention has shifted to polar textures that arise in ferroelectric crystals [9–11]. In such systems, the driving forces are the anisotropy of the local electric dipoles and their coupling to lattice distortions, rather than DMI. Polar skyrmions were first identified in ferroelectric/paraelectric multilayers [10,11], following the observation of polar vortices in $\text{PbTiO}_3/\text{SrTiO}_3$ superlattices [12,13]. Since then, an increasing number of purely ferroelectric materials have now been predicted, or even observed, to harbor nontrivial topology [14–20]. Prominent examples include “skyrmion bubbles” in PbTiO_3 [18] obtained from molecular-dynamics (MD) simulations. Complementary progress includes the discovery of emergent topological

polarization textures (vortices/merons) in lead-based relaxor ferroelectrics such as PMN-PT [21] and the experimental imaging of meron–antimeron networks in moiré ferroelectrics based on twisted vdW bilayers [22]. Especially intriguing for the present work is the theoretical prediction that bulk barium titanate (BaTiO_3 , BT) in its rhombohedral phase can sustain a variety of polar textures. Gonçalves *et al.* [20] showed that antiskyrmions with a topological charge of -2 can be created by locally inverting the polarization. In subsequent studies, it was demonstrated that the same objects can be written and steered with external electric fields [14], and that one-dimensional (1D) line defects [17] (skyrmion lines) are also possible. Although most -2 antiskyrmion calculations were performed at cryogenic temperatures, previous work [15] revealed theoretical thermal stability up to ~ 85 K. More recently, Gómez-Ortiz *et al.* [16] proposed electrically switchable skyrmion–antiskyrmion tubes with $Q = \pm 1$ in rhombohedral BT. Beyond electric-field control, structured light has recently been proposed to manipulate ferroelectric topologies, including dynamical polar (anti)skyrmions and chirality selection [23].

Beyond their mere existence, the internal structure of the -2 antiskyrmions is remarkable. For diameters below ~ 4 nm, the topological charge density is fragmented into six hotspots carrying $-1/3$ each, entities denoted as topological quarks [15,20]. They exhibit well-defined positions, charges and quasiparticle-like behavior. When the diameter exceeds ~ 4.5 nm every $-1/3$ quark splits into two $-1/6$ pre-quarks while the global symmetry and net charge are preserved

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[15]. The nontrivial topology is thus concentrated at the antiskyrmion vertices, whereas the regions in between relax into a trivial 180° domain wall [15]. These observations already portray BT as an ideal playground for exploring how topology evolves with size and dimensionality. Topological objects with $|Q| > 1$ are not merely academic curiosities [24–26]. A larger net charge magnifies the emergent electromagnetic fields and promises stronger electro-optic responses as well as genuine multilevel states for nonvolatile memories. Hosting positive and negative charges in the same crystal would further allow domain-engineered conduits for topological currents and offer a solid-state analogue of confinement phenomena usually discussed in high-energy physics. These considerations motivate the search for systems in which possible skyrmion and antiskyrmion textures can coexist and interact.

With this objective in mind, and motivated by the already rich set of predicted topological textures in pure BT, we extend our study to investigate the effects of substituting Ti with Zr, i.e., barium zirconate titanate $[\text{Ba}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3]$, BZT. The motivation arises from the BZT phase diagram (Refs. [27–29]), which shows that with an appropriate choice of Zr concentration, the rhombohedral phase can be stabilized above room temperature. This rhombohedral structure is precisely the prerequisite for the topological textures previously induced in pure BT [14,15,20]. The relevant concentration range for this large stabilizing effect of the rhombohedral phase lies around 10–15% Zr [27]. In this study, we carry out finite-temperature molecular dynamics (MD) simulations using a first-principles parameterized effective Hamiltonian [27] for BZT, computational details are provided in the next section. First, we study a high-symmetry ordered 12.5% Zr arrangement in which the B-site lattice is doubled along each Cartesian direction (period two), yielding one Zr per doubled cell and a $1/8$ overall substitution. In this system, we again induce nanodomains [15,20] and find that stable topological textures persist. Remarkably, because of the doubling of the unit cell introduced by chemical substitution, the well-known charge -2 antiskyrmion [14,15,20] undergoes a splitting. More specifically, the doubled unit cell separates into two topologically distinct regions: one half hosts the previously reported -2 antiskyrmion composed of six $-1/3$ topological quarks, while the other half hosts a $+4$ skyrmion with six $+2/3$ quarks. This behavior mainly originates from the underlying chemical sublattice and the accompanying change in local anisotropy. In addition to the real-space analysis, we introduce an optional symmetry-based bookkeeping perspective for the chemically doubled stacking and show that the $+1$ -per-vortex offset is mediated by localized interfacial core-conversion events. Next, we examine whether stable topological textures can also be sustained in systems with randomly distributed Zr ions. We find that nontrivial topological textures remain robust under random substitution of Zr. However, with increasing Zr concentration, these textures become distorted and deviate from the highly symmetric configuration. All of these simulations are carried out at low temperature (1 K). We then address the intrinsic thermal stability of these textures and find that, depending on concentration, they can remain stable up to nearly 100 K. Finally, we take one step further and demonstrate that in the 12.5% superlattice, topological textures can also be induced

near room temperature by applying external electric fields, although their stability requires the continued presence of the field.

Overall, this work presents a comprehensive study of topological textures in Zr-substituted BT. We show that chemical substitution not only preserves but also enriches the zoo of emergent textures by enabling unit-cell doubling, which gives rise to an interplay of fractionalized topological charges ($-1/3$ and $+2/3$ quarks). We further demonstrate that these textures remain robust under random substitution, can be stabilized up to nearly 100 K, and, with the aid of external electric fields, can even be induced at room temperature.

II. COMPUTATIONAL DETAILS

In this study, the computational experiments were performed using MD simulations based on effective Hamiltonians (EH) [28,30–36]. Effective Hamiltonians provide the advantage of being highly efficient [37] while still delivering a reliable, quantitative description of the underlying atomistic effects [36,38]. The parametrizations employed here were developed in the works of Mayer *et al.* [27,38], incorporating anharmonic couplings for pure BT as well as an improved treatment of substitution effects. More details on the Hamiltonian for pure BT can be found in Ref. [38], while the Hamiltonian applied for Zr-substituted BT is comprehensively described in Ref. [27]. For completeness, a summary of the model and notation is provided in the Supplemental Material [39]. Within this EH framework, the microscopic order parameter is a B-site-centered local mode vector $\mathbf{u}(\mathbf{R})$ defined for each five-atom perovskite unit cell. It is directly associated with the corresponding local dipole moment $\mathbf{d}(\mathbf{R}) = Z^*(\sigma_{\mathbf{R}})\mathbf{u}(\mathbf{R})$, where $Z^*(\sigma_{\mathbf{R}})$ is the (species-dependent) mode Born effective charge [27,39] of the B-centered unit cell at site $\mathbf{R}$. The local polarization is then $\mathbf{p}(\mathbf{R}) = \mathbf{d}(\mathbf{R})/\Omega_0$, with Ω_0 the unit-cell volume. For topology, we use the normalized order-parameter field $\mathbf{n}(\mathbf{R}) = \mathbf{u}(\mathbf{R})/|\mathbf{u}(\mathbf{R})|$ [equivalently $\mathbf{n}(\mathbf{R}) = \mathbf{p}(\mathbf{R})/|\mathbf{p}(\mathbf{R})|$]. Another clear advantage of these parametrizations is their accurate description of phase transition temperatures for both pure and substituted BT [27,38], which ensures meaningful and reliable simulation results. All simulations were carried out using a modified version of the *feram* software [34,35]. The simulations were conducted in the canonical ensemble, with temperature scaling achieved using a velocity-scaling algorithm, validated against Nosé-Poincaré [40] results. A timestep of 2 fs was employed for all simulations. Each trajectory ran for 1 ns (800 ps equilibration + 200 ps production). The simulation cell was fixed at $64 \times 64 \times 64$ unit cells with periodic boundary conditions in all three directions employed. For disordered BZT, we performed three independent simulations with randomized B-site occupations to assess statistical variability and mitigate seed-specific effects.

For characterizing topological textures within our study, we utilize the Pontryagin density [see Eq. (1)], which quantifies the topological charge for a continuum unit-vector order-parameter field $\mathbf{n}(\mathbf{r})$ defined over a two-dimensional spatial domain (compactified to S^2) and mapping into the two-sphere target space S^2 , corresponding to the homotopy group $\pi_2(S^2) = \mathbb{Z}$.

For the actual computation of the topological charges Q , we use the lattice formulation proposed by Berg and Lüscher [41], as illustrated in the work of Heo *et al.* [42]. In the latter work, the lattice discretization is given in Eqs. (2) and (3). The summation is carried out over the areas A_l of the spherical triangles spanned by the vectors $\mathbf{n}_i$, $\mathbf{n}_j$, and $\mathbf{n}_k$, where $\mathbf{n}_i \equiv \mathbf{n}(\mathbf{R}_i)$ denotes the normalized order-parameter field on lattice site i . Here, the spin vectors of Ref. [42] are replaced by the corresponding normalized vectors constructed from the effective-Hamiltonian local modes (or equivalently the local polarization field). The sign is determined by the relation $\text{sign}(A_l) = \text{sign}[\mathbf{n}_i \cdot (\mathbf{n}_j \times \mathbf{n}_k)]$,

$$Q = \frac{1}{4\pi} \int_{\Omega} \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n}) d^2 r \quad (1)$$

$$Q = \frac{1}{4\pi} \sum_l A_l \quad (2)$$

$$\cos\left(\frac{A_l}{2}\right) = \frac{1 + \mathbf{n}_i \cdot \mathbf{n}_j + \mathbf{n}_j \cdot \mathbf{n}_k + \mathbf{n}_k \cdot \mathbf{n}_i}{\sqrt{2(1 + \mathbf{n}_i \cdot \mathbf{n}_j)(1 + \mathbf{n}_j \cdot \mathbf{n}_k)(1 + \mathbf{n}_k \cdot \mathbf{n}_i)}} \quad (3)$$

III. RESULTS

A. Alternating $-2/+4$ textures in a chemically doubled unit cell

Since the existence of -2 antiskyrmions in BT relies on the rhombohedral phase [20] (R3m), we begin by constructing a system that preserves the crystallographic prerequisites for such textures and thus may also host nontrivial topology. For Zr-substituted BT, we must remain in the concentration range where the rhombohedral phase is stable. The BZT phase diagram (Refs. [27–29]) shows that the transition temperature from rhombohedral to orthorhombic symmetry initially increases with Zr concentration, reaching a maximum at about 10–15% where it exceeds 300 K, before decreasing again at higher substitution levels. We therefore choose 12.5% and construct a $2 \times 2 \times 2$ cell, where one Ti ion is replaced by Zr, yielding the desired composition. To assess whether the superlattice satisfies the basic prerequisites for hosting topological textures, we performed initial first-principles density-functional theory (DFT) calculations [43–48]. These show that the superlattice adopts a rhombohedral ground state with spontaneous net polarization along [111], providing the crystallographic setting required for the textures reported in pure BT. We also computed the spontaneous polarization and compared it with results from our EH simulations (see Fig. S1 with in the Supplemental Material [39]). The two approaches exhibit reliable quantitative agreement (within the numerical uncertainty of the EH parametrization). Importantly, despite the presence of nominally nonpolar Zr-centered cells, the superlattice retains a substantial net polarization. Together, these findings indicate that the structural and polar conditions necessary to stabilize topological textures, analogous to those in pure BT, are indeed met in the 12.5% Zr superlattice. More details on these calculations and of this superlattice is provided in the Supplemental Material [39]. With an effective Hamiltonian for BZT available [27], we can now perform large-scale MD simulations [27,37]. We follow the procedure of Ref. [15] and consider a $64 \times 64 \times 64$ supercell with Zr distributed as described above. Initially, we restrict ourselves to a low temperature of 1 K. To induce nanodomains, the

supercell is first initialized as a single domain with polarization along [111]. We then invert the polarization within approximately cylindrical regions aligned with [111], effectively creating nanodomains with circular cross section. This serves as the starting configuration: From here, the MD simulation is allowed to evolve freely so that the system can relax. In this superlattice we introduce nanodomains with diameters ranging from ~ 2.2 to ~ 10 nm. The system is equilibrated for 800 ps at 1 K, and results are averaged over a subsequent 200 ps. We find that nanodomains with diameters between ~ 3 and ~ 10 nm remain stable, while the smallest domain (~ 2.2 nm) decays into a single-domain state within a few tenths of picoseconds. Thus, as in pure BT, stable nanodomains are formed in the 12.5% BZT superlattice. The central question is now whether these nanodomains also host nontrivial topological textures. To answer this, we analyze cross sections in planes normal to the nanodomain axis, i.e., the (111) planes. Here, an additional symmetry consideration becomes important. In the undoubled lattice, there are three symmetry-distinct (111) planes per period along [111], analogous to ABC stacking in fcc. This trio constitutes the fundamental geometric unit of the texture. In the present case, chemical substitution doubles the unit cell along [111]. While the geometric stacking remains unchanged, the chemical motif alternates, resulting in two inequivalent halves: one with Ti–Zr–Ti stacking and the other with Zr–Ti–Zr. In other words, the chemical motif is reversed between the two halves of the doubled unit cell. For the analysis of topological textures, we therefore work with the three symmetry-distinct geometric (111) planes that constitute the topological unit, whereas the alternating chemical motif acts as a background modulation and does not redefine these planes. Consequently, unlike in previous studies [15,20], two distinct (111) projections must be considered because of the doubled unit cell along [111].

We now proceed with our initial analysis. Following Sec. II, we compute the plane-resolved topological charge for projections onto the (111) planes in geometric triplets. Specifically, at each position z' we define the plane-integrated topological charge (slice charge) as $Q(z') = \int q(x', y'; z') dx' dy'$, where $q(x', y'; z')$ is the local topological charge density on the (111) plane at fixed z' [see Eq. (1) for the Pontryagin density and Eq. (3) for its lattice evaluation]. We then translate the projection window along the nanodomain axis and repeat. The axial direction z' is defined by rotating the simulation cell so that z' is parallel to [111]. The resulting $Q(z')$ is shown in Fig. 1(a). Each data point corresponds to a single (111) plane, so that three consecutive points form one geometric triplet along z' .

A striking alternation emerges. One half of the chemically doubled unit cell (shaded region) hosts the familiar -2 antiskyrmion known from pure BT [20], whereas the other half hosts a $+4$ skyrmion. This $-2/+4$ pattern repeats periodically along the nanodomain (z') direction. To compare the real-space textures, Figs. 1(c) and 1(d) display the (111)-plane projections of the two halves using the rotated in-plane axes $x' || [1\bar{1}0]$ and $y' || [11\bar{2}]$. We also plot the local topological charge density $q(x', y'; z')$. Both patterns in Figs. 1(c) and 1(d) exhibit a hexagonal-like in-plane dipole arrangement on (111), consistent with the parent 3m point group symmetry

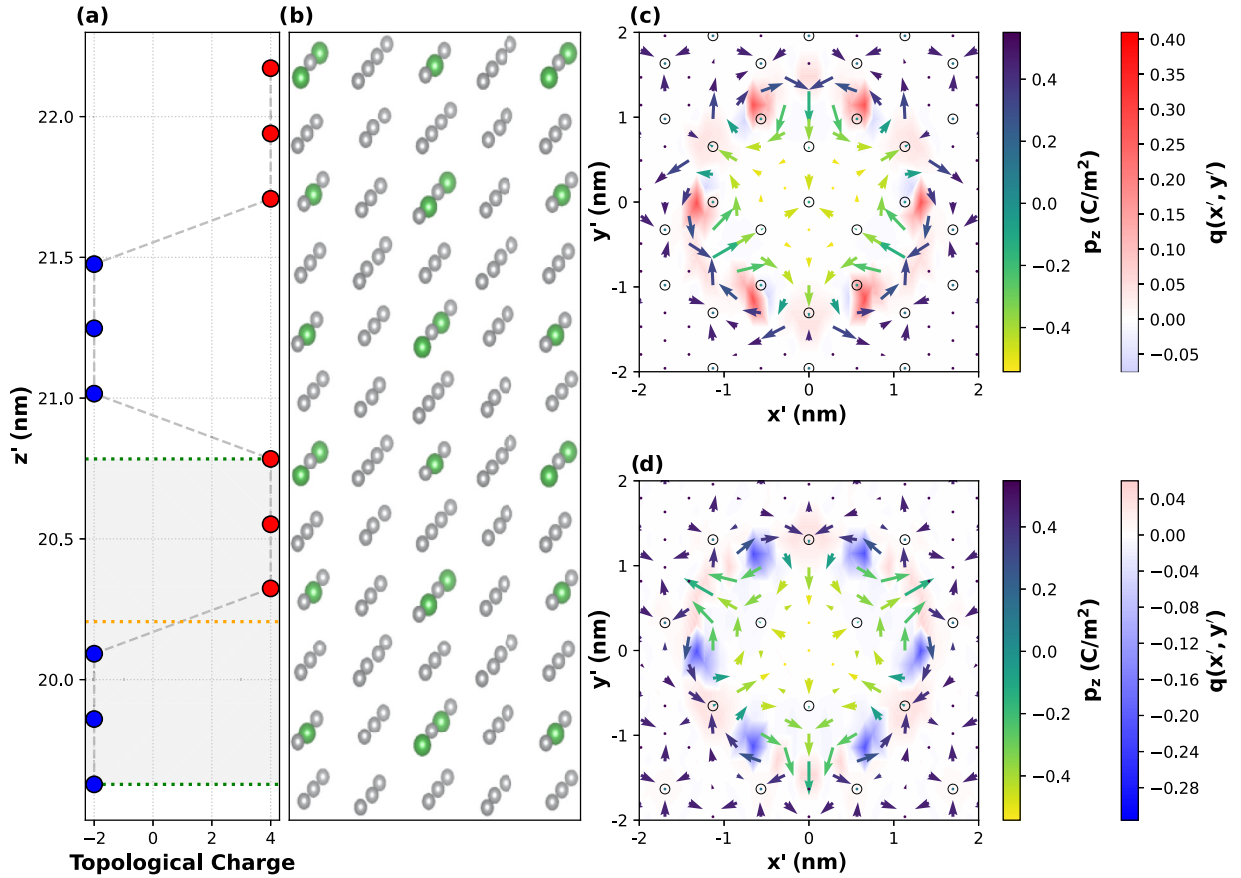


FIG. 1. Topological behavior in the 12.5% superlattice along the nanodomain axis z' . (a) Integrated topological charge along z' along the [111] direction. The shaded region marks the chemically doubled unit cell, and the orange line indicates the chemical interface associated with the change in topological character. (b) Schematic associated B-site ordering: gray (smaller) spheres indicate Ti ions, and green (larger) spheres represent Zr ions. (c) Local polarization vectors of the $Q = +4$ skyrmion, colored by the out-of-plane component. The overlaid local topological charge density reveals its fragmentation into six $+2/3$ topological quarks. (d) The $Q = -2$ antiskyrmion, similarly decomposed into six $-1/3$ topological quarks. Panels (c) and (d) are shifted along z' relative to each other, consistent with the offset seen in (a). In the latter panels, small circles indicate Zr-substituted unit cells.

[15,20]. In Fig. 1(d), the -2 antiskyrmion (diameter ~ 3 nm) comprises six vortices with alternating clockwise and counterclockwise circulation, together with three vertices where the in-plane polarization diverges outward and three where it converges inward, fully consistent with pure BT [14,15,20]. Each vortex coincides with a hotspot of $q(x', y'; z')$ carrying approximately $-1/3$, yielding six $-1/3$ topological quarks. By contrast, Fig. 1(c) shows that the $+4$ texture retains the same six-vortex scaffold (threefold motif), but the polarization texture around the individual cores differs measurably from the -2 half; interestingly, the hotspots now carry $+2/3$. The $-1/3$ and $+2/3$ hotspots occur in the same six angular sectors [see Figs. 1(c) and 1(d), and also Fig. S2 within the Supplemental Material [39]], indicating that the global six-vortex scaffold and $3m$ symmetry are preserved, while the core-level geometry differs and the fractional charges shift.

We can interpret these results as follows: The alternation of -2 and $+4$ textures originates from the two-sublattice chemical motif introduced by Zr substitution, which doubles the unit cell along [111]. Although the geometric stacking of planes is unchanged, the chemical motif is reversed between the two halves ($\text{Ti-Zr-Ti} \leftrightarrow \text{Zr-Ti-Zr}$). This reversion modifies the local anisotropy landscape and, effectively,

the coefficients of the gradient-like terms (in the EH sense of composition-dependent short-range couplings [27]) on alternating (111) planes. As a result, the plane-resolved skyrmion density acquires an integer offset when passing from one half to the other: Each vortex's fractional charge changes from $-1/3$ to $+2/3$, i.e., by $+1$. Summing over the six vortices therefore shifts the total from -2 to $+4$ while preserving the texture's morphology: $-2 + 6 \times (+1) = +4$.

The $-2/+4$ alternation emerges directly from how the slice-resolved skyrmion density redistributes across the chemically doubled cell. In real space, the inter-half difference map $dq(x', y')$ shows localized peaks at the vortex cores while the six-vortex scaffold remains trackable across the interface. Integrating dq over each peak yields an approximately integer $+1$ per vortex line (total $\Delta Q \approx +6$ per half-cell), with vortex positions and overall $3m$ point group symmetry essentially unchanged (see the Supplemental Material [39]). The chemical interface therefore acts as an effective conduit of topological charge that converts the local fractional assignments on each slice (e.g., $-1/3$ to $+2/3$ on matching vortex cores) without requiring lateral motion of the cores.

Two immediate consequences follow: (a) the $-2/+4$ sequence constitutes a topological charge-density wave along

z' whose wavelength is fixed by the chemically doubled periodicity, (b) because the six vortex scaffold is nearly invariant through the interface, the switching of fractional charge is governed primarily by the layer-dependent anisotropy set by the chemical sublattice, offering a route to engineer fractionalization via compositional anisotropy modulation rather than by altering nanodomain geometry.

The splitting of the topological texture described above is observed for nanodomain diameters up to approximately 4.5 nm. For larger diameters, the system exhibits the previously reported splitting [15] of the topological quarks (e.g., from $-1/3$ into $-1/6$), and the broadened cores sample multiple low- $|p|$ sites, which blurs the clean $-2/+4$ alternation and produces more complex patterns that we do not pursue further here. In the next section, we provide an optional symmetry-based bookkeeping perspective for the observed integer offset between the two chemical halves and discuss its microscopic realization via localized core-conversion events.

B. Symmetry bookkeeping and microscopic charge-transfer mechanism

As an optional view alongside the real-space narrative, we can model the chemically doubled unit cell along $z' || [111]$ as a static binary background. The two halves (Ti–Zr–Ti and Zr–Ti–Zr) can be considered as an Ising-like “color” field with $\mathbb{Z}_2$ link variables that are $+1$ within a half-cell and flip sign across the chemical interface. In this notation, a half-cell translation along z' corresponds to a fixed sign change, whereas a full-cell shift is ordinary. We emphasize that this construction is optional and does not enter the quantitative analysis of Sec. III A, it is offered solely as a compact language for discussing symmetry and phase conventions imposed by the chemical doubling.

In this language, the color-sensitive quantity is a phase-like variable that records the in-plane rotation of the polarization relative to a chemically anchored reference frame. Crossing the chemical interface applies a fixed 180° flip to that reference frame, so this variable changes sign between the two halves, even though the polarization pattern can evolve continuously with the local anisotropy. This background-imposed sign convention partitions adjacent planes into inequivalent bookkeeping sectors and provides a compact description of the observed alternation.

Analyzed plane by plane along z' , one half of the doubled cell carries a plane-integrated topological charge of -2 , while the other carries $+4$. In our topological quark language, the -2 texture decomposes into six $-1/3$ quarks, whereas the $+4$ texture decomposes into six $+2/3$ quarks at essentially the same in-plane positions. The color background provides a compact description: A half-translation corresponds to a fixed $\mathbb{Z}_2$ phase convention (a π reference-frame flip) between the two chemical halves, which provides compact bookkeeping for the observed $+1$ -per-vortex offset. Summing over six aligned vortices shifts -2 to $+4$ while preserving the six-vortex scaffold (coincident vortex-axis positions), even though the core-resolved polarization textures differ between the two halves.

Regarding how the integer offset is realized microscopically, a change of the plane-resolved skyrmion number

requires a breakdown of the normalized order-parameter field $\mathbf{n}(\mathbf{R})$ [i.e., $\mathbf{n}(\mathbf{R}) \equiv \mathbf{p}(\mathbf{R})/|\mathbf{p}(\mathbf{R})|$, equivalently $\mathbf{u}(\mathbf{R})/|\mathbf{u}(\mathbf{R})|$], a singular event in the local-mode texture. In our data, the six vortex cores remain approximately axially aligned across the chemical interface, while $|\mathbf{p}|$ becomes strongly suppressed at the vortex axis within the interfacial region (see Figs. S2 and S3 within the Supplemental Material [39]), consistent with Bloch-point-like polarization singularities (local $|\mathbf{p}| \rightarrow 0$) [49–51]. Microscopically, such nodes are naturally facilitated by Zr-centered cells: Compared with Ti-centered environments, Zr substitution yields locally “softer” polar response and can support configurations with very small local polarization amplitude. This provides chemically available sites at which the vortex axis can transiently extinguish $|\mathbf{p}|$, enabling the required integer jump in the plane-resolved topological charge without lateral motion of the vortex cores. In this sense, the interface acts as a chemically assisted conversion region, where Bloch-point-like nodes serve as local sources/sinks of topological density and transfer one integer unit per vortex line between adjacent (111) sections. The $\mathbb{Z}_2$ construction above serves as optional bookkeeping for this integer offset, the microscopic conversion is mediated by the localized singular cores described here.

Two internal checks are consistent with this picture: (a) the plane-resolved $Q(z')$ from Fig. 1(a) exhibits a clean $-2/+4$ alternation within a single nanodomain, (b) subtracting the local topological charge densities of the two halves yields six coincident peaks, each integrating to approximately $+1$, i.e., one unit gained per quark, under the $\mathbb{Z}_2$ bookkeeping convention. The latter check is provided in Fig. S4 within the Supplemental Material [39]. This proposed organizing principle presumes that corresponding vortex cores remain approximately axially aligned along z' (as observed for diameters below ~ 4.5 nm). Strong disorder or lateral wandering can already blur the alternation. In addition, as the skyrmion diameter increases and the vortex cores broaden, the number of Zr-centered cells sampled within a given core increases, providing multiple low- $|p|$ candidate sites for singular conversion events; this can delocalize the charge-transfer process along z' and degrade the clean $-2/+4$ alternation within a single nanodomain. In that regime, a purely real-space description is more appropriate. Within its range of validity, the color background provides a compact, alternative field-theoretic lens on the observed $-2 \rightarrow +4$ sequence.

C. Topological textures in randomly substituted BZT

Having established that nontrivial topological textures can be induced in the highly symmetric 12.5% superlattice, we now turn to a more experimentally accessible scenario: random Zr substitution. Our protocol (nanodomain induction, supercell size, MD settings, and plane-resolved analysis) is identical to the superlattice case. The only change is the composition: We distribute Zr ions at random in steps of 2% from 0% (pure BT) up to 12.5% within the simulation box. We focus on an induced nanodomain of diameter ~ 4 nm and fix the temperature at 1 K. Overall, for all simulated compositions, nanodomains can be created and remain stable over the full simulation window. Figure 2 summarizes

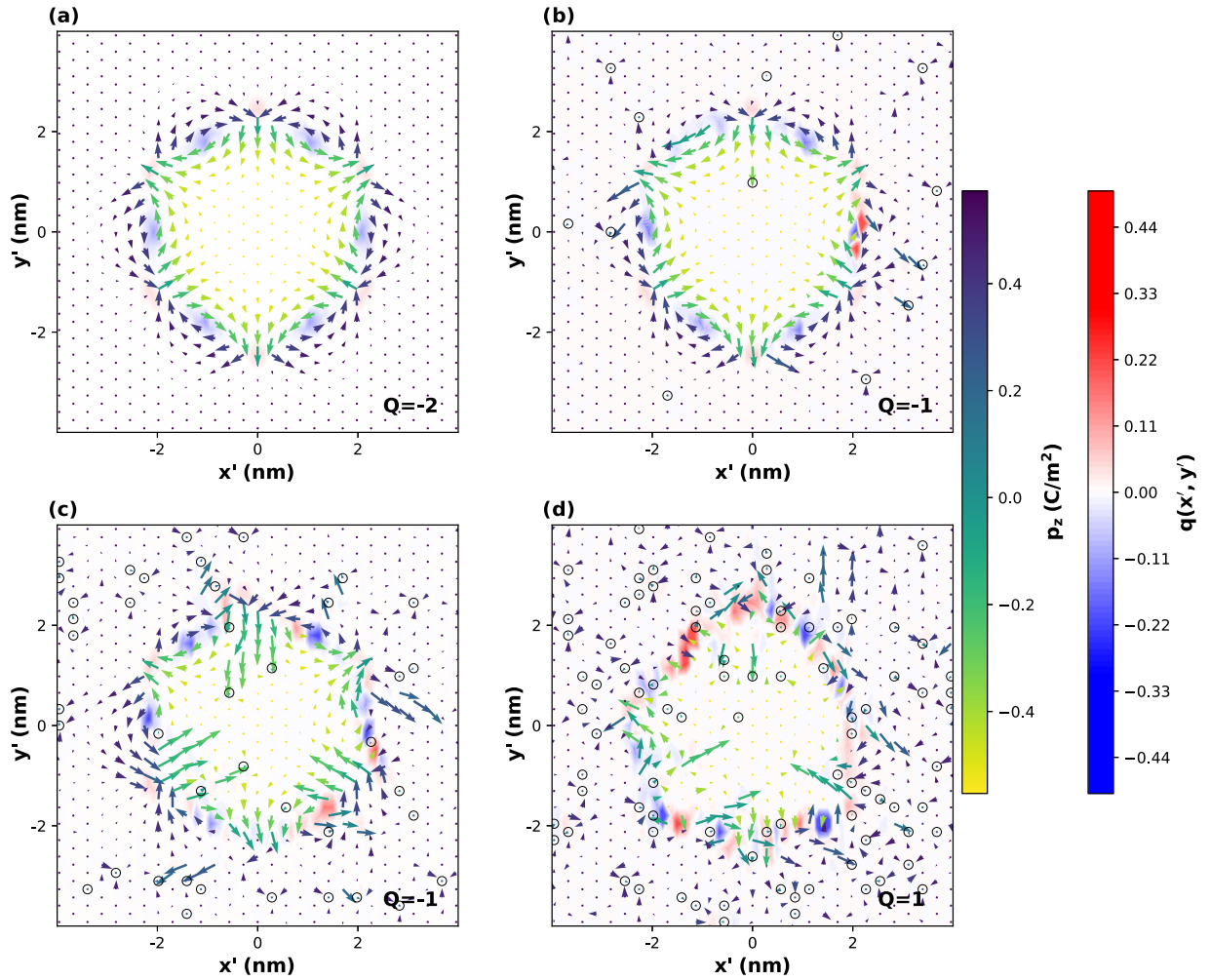


FIG. 2. Topological textures in random BZT. Each panel shows the in-plane polarization vectors in the (111) projection, color-coded by the out-of-plane component, with the local topological charge density overlaid. (a) Pure BT, displaying the canonical $Q = -2$ antiskyrmion. (b) 2% randomly distributed Zr, showing the same underlying texture with minor defects. (c) 6% randomly distributed Zr, where defects become more pronounced but the overall symmetry is still largely preserved. (d) 12.5% randomly distributed Zr, exhibiting strong deviations and fragmentation of the topological charge into multiple pieces, while still retaining a coarse imprint of the original symmetry. In all panels, small circles indicate Zr substituted unit cells.

the associated topological textures using a single projection along z' . In the absence of imposed chemical doubling, this serves as a first indicator rather than a full 3D characterization. Nevertheless, because Zr ions are distributed randomly, the textures do show variations along the nanodomain axis. In Fig. 2(a) (0% Zr), pure BT reproduces the canonical -2 antiskyrmion with its six-vortex scaffold and the familiar threefold rotational symmetry. The plane-resolved topological charge remains essentially constant at $Q = -2$ along the nanodomain. In Fig. 2(b) (2% Zr), the global threefold symmetry is still preserved, but local anisotropy fluctuations introduced by isolated Zr ions distort individual vortices. In the local charge density $q(x', y'; z')$, this manifests as a positive hotspot at one vortex core. As a result, the plane-integrated charge for that section is reduced to topological charge of -1 instead of -2 . This demonstrates that local defects can modify the topological charge while leaving the global six-core scaffold and threefold motif recognizable. At 6% substitution [Fig. 2(c)], disorder effects become more pronounced. Vortex cores exhibit pinning and shear, so the threefold symmetry

remains visible at the mesoscopic scale but is clearly broken locally. The charge density $q(x', y'; z')$ displays both positive and negative hotspots of varying strength. In several regions, we observe partial conversion events in which only subsets of vortices undergo charge transfer, leading to irregular fluctuations of $Q(z')$ (see Fig. S5 within the Supplemental Material [39]) along the nanodomain axis. At the highest investigated concentration, 12.5% [Fig. 2(d)], the nanodomain remains remarkably robust, and a nontrivial texture is still sustained. The pattern resembles a patchwork version of the pure case, with a reduced correlation length: multiple hotspots appear at the characteristic scaffold positions, yet the six-vortex framework is still recognizable. The plane-resolved charge $Q(z')$ (see Fig. S5 within the Supplemental Material [39]) varies significantly along the axis and frequently deviates from the canonical $Q = -2$ value of pure BT, indicating that the texture remains topologically nontrivial and strongly modulated by compositional disorder.

We can interpret these results as follows: Random Zr substitution introduces quenched anisotropy and random-field

disorder that significantly influence the stability and morphology of the textures. First, local variations in the chemical environment pin and bend vortex lines, leading to distortions of the otherwise symmetric vortex scaffold. Second, these variations generate narrow interfacial regions where the local topological charge density $q(x', y'; z')$ changes abruptly, thereby enabling charge transfer between neighboring planes (see the Supplemental Material [39]). Third, such processes give rise to a spatially heterogeneous redistribution of fractional charges: vortices carrying $-1/3$ in pure BT can locally convert into $+2/3$, combine to larger fractions, or split into smaller fractions, depending on the local arrangement of Zr ions. The emergent state can thus be viewed as a skyrmion-glass-like texture pinned by quenched disorder, by analogy with magnetic skyrmion glasses [52,53]. The six-vortex scaffold characteristic of the -2 texture remains broadly recognizable, but its internal fractionalization is strongly modulated by compositional randomness. Because these charge-transfer events occur irregularly along the nanodomain axis, the system cannot be unambiguously classified into a single texture type (e.g., -2 or $+4$) as in the ordered superlattice. Instead, the textures acquire a patchwork character, with local motifs resembling fragments of the ordered cases embedded in a disordered background.

D. Intrinsic thermal stability vs Zr concentration

So far, our simulations have been performed at very low temperature (1 K), where nanodomains and their associated topological textures are stable. For experimental relevance and prospective applications, we now assess thermal stability. Following Ref. [15], we probe the intrinsic stability by ramping the temperature in MD while monitoring the plane-resolved topological charge Q . Specifically, we initialize three different nanodomains (~ 3.5 , ~ 5 , and ~ 6.5 nm) at 1 K, then increase the temperature in 5 K steps until collapse. The collapse temperature T_{collapse} is defined as the temperature at which the nanodomain irreversibly collapses into a single-domain state under our simulation protocol. We perform such heating runs for random Zr concentrations from 0% to 12.5% (in 2% steps) and for the 12.5% superlattice. For all presented results, only one (111) projection is used to compute the topological charge in Figs. 3(a)–3(c); however, as noted earlier (Fig. S5 within the Supplemental Material [39]), randomness of the Zr distribution also induces fluctuations of Q along the core.

We first examine how the plane-resolved topological charge evolves with temperature. As noted above, we consider three nanodomain diameters across random Zr concentrations and in the 12.5% superlattice. Figures 3(a)–3(c) summarize these results. For pure BT, all three diameters retain the canonical -2 texture over almost the entire temperature range up to T_{collapse} , consistent with Ref. [15]. In the superlattice, the behavior is likewise nearly constant. That means for the 3.5 nm domain the alternating $-2/+4$ pattern persists also to finite temperature (even up to T_{collapse}), whereas for 5 nm and 6.5 nm the alternation has vanished and the topological texture along z' constantly shows the -2 behavior. [Figure 3(a) displays only the -2 branch for the superlattice because a single (111) projection along z' is analyzed.]

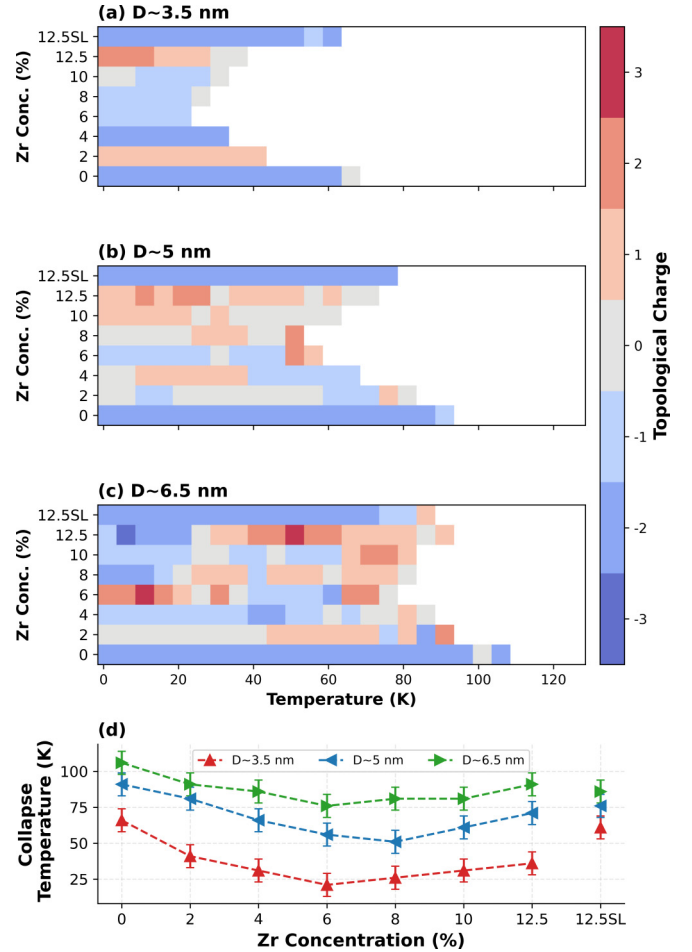


FIG. 3. Intrinsic thermal stability of nanodomains, and the associated topological textures, as a function of composition and temperature. (a) Evolution of the integrated topological charge with temperature for an induced diameter D of ~ 3.5 nm. (b) Same as (a) for ~ 5 nm. (c) Same as (a) for ~ 6.5 nm. (d) Collapse temperature (T_{collapse}) (averaged over three independent runs) as a function of Zr concentration for the three studied diameter scenarios. “12.5SL” denotes the 12.5% ordered superlattice.

For randomly Zr-substituted systems, the behavior changes qualitatively. Already at 2% Zr, fluctuations in the topological charge appear upon heating. Nevertheless, nanodomains remain topologically nontrivial throughout their thermodynamic stability window. We note that $Q = 0$ in a given (111) slice does not necessarily imply a trivial texture, since positive and negative fractional contributions can cancel in the plane integral while a nontrivial vortex scaffold remains present. With increasing Zr content, the fluctuations grow, and occasional excursions to more exotic integer values are observed, although such events are rare, instead the predominant values lie between -2 and $+2$. These trends again indicate that Zr introduces local anisotropy variations that distort and pin the vortex skeleton, producing a heterogeneous, disorder-modulated sequence of plane textures. In short, random substitution induces charge fluctuations upon heating and along z' , yet the nontrivial character persists until the nanodomains eventually collapse.

Figure 3(d) explicitly illustrates the collapse temperatures as a function of diameter and composition. In detail, for each concentration, we performed three independent heating runs with randomly distributed Zr, that means we report the mean T_{collapse} across these runs and estimate the uncertainty from their spread. For pure BT, increasing diameter modestly enhances stability. That means we obtain a T_{collapse} of ~ 65 K for 3.5 nm and ~ 110 K for 6.5 nm (the 5-nm case lies in between), in agreement with Ref. [15]. With random Zr, the T_{collapse} decreases for all diameters, most strongly for 3.5 nm and less strongly as the diameter grows. A minimum occurs near 6–8% Zr, after which T_{collapse} recovers slightly toward 12.5%. In the superlattice, the T_{collapse} indicates a reduced dependency on the diameter. Interestingly, at 12.5% Zr and 6.5 nm the random composition displays a slightly higher T_{collapse} than the superlattice. For higher Zr contents ($\leq 15\%$), nanodomains can still be stabilized at 1 K but fragment into multidomain states upon heating, consistent with the progressive weakening of the ferroelectric instability under enhanced substitution.

At first glance, the bulk BZT phase diagram [27–29] suggests that increasing Zr toward $\sim 12.5\%$, which raises the rhombohedral–orthorhombic (R–O) transition temperature, should monotonically stabilize the nanodomains. In practice, the nanodomain collapse temperature does not track the bulk R–O line: interfacial energetics and disorder dominate. These trends can be interpreted as follows. Average softening with Zr reduces ferroelectric stiffness and the effective domain-wall energy, driving the initial drop in T_{collapse} . With further substitution, disorder pinning and self-averaging counterbalance this softening, meaning quenched compositional disorder both hinders wall motion and becomes more homogeneous on mesoscopic scales, yielding the partial recovery near 12.5%. Finally, finite-size effects favor larger cylinders because the tendency of a cylindrical domain wall under tension to contract becomes weaker with increasing radius, and larger domains interact with a wider range of pinning centers. Together, these effects suppress thermally driven shrinkage and increase T_{collapse} . This also explains why, at large diameter, the random 12.5% composition can slightly outperform the superlattice: For extended walls, a distributed pinning landscape can provide a higher effective barrier to collapse than the coherent soft modes accessible in a periodic modulation.

Overall, pure BT offers the highest intrinsic stability. Zr substitution generally reduces it, albeit with a composition window where disorder-assisted pinning compensates. Larger diameters are systematically slightly more robust. Importantly, nontrivial topology persists over broad temperature ranges even in random BZT up to 12.5% Zr.

E. Field-stabilized topological textures near room temperature

Finally, we ask whether ferroelectric nanodomains with nontrivial topology can be stabilized near room temperature. The previous section showed intrinsic thermal stability windows of ~ 50 – 100 K (depending on Zr content and ordering), a clear improvement over the ~ 1 K range of our initial studies, but still insufficient for practical applications. Our focus here is the realization and control of such textures around 300 K. To address the prerequisite, rhombohedral stability near 300 K,

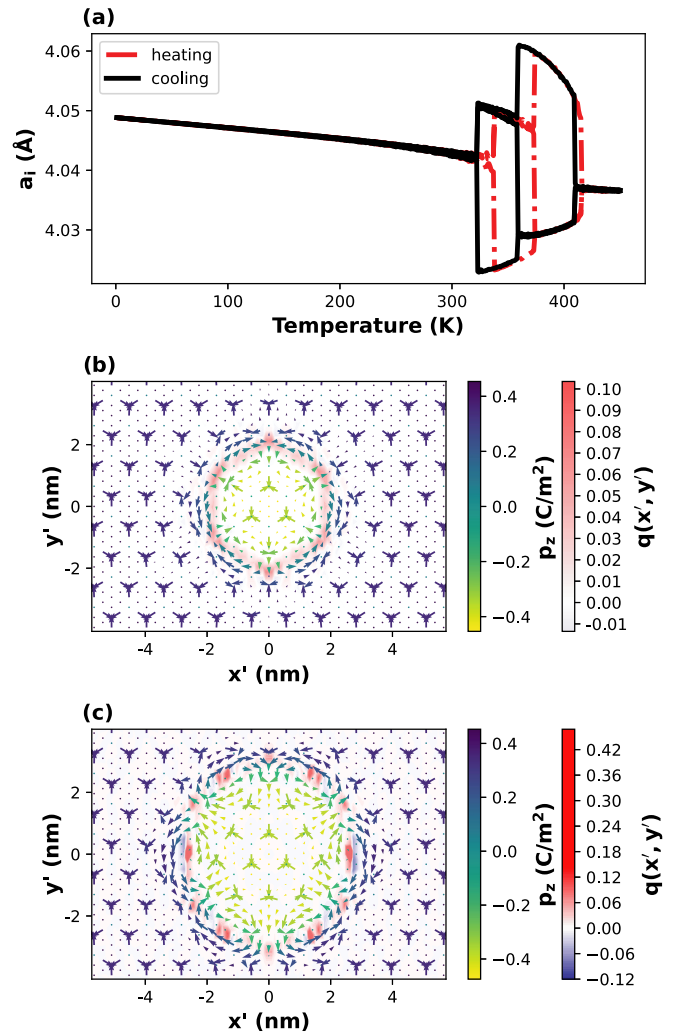


FIG. 4. Phase behavior and near room-temperature field-induced stabilization of nanodomains in the 12.5% ordered superlattice. (a) Phase diagram of the 12.5% superlattice (in terms of the lattice parameters a_i), showing rhombohedral stability above 300 K. (b) Skymion with charge $Q = +4$ and a diameter of ~ 4 nm, written and stabilized at 293 K under a local electric field of 350 kV/cm. (c) Larger $Q = +4$ skymion with a diameter of ~ 6 nm under the same conditions. Panels (b) and (c) use the (111) projection, with in-plane polarization vectors color-coded by the out-of-plane component and the local topological charge density overlaid. In both cases, fragmentation of the topological charge is observed.

we first computed the finite-temperature phase diagram of the 12.5% superlattice (using the same $64 \times 64 \times 64$ cell and Zr configuration as before), heating from 1–450 K in 1 K steps and cooling symmetrically. Figure 4(a) (illustrating the lattice parameters vs temperature) shows that all four BT-like phases persist, but shifted relative to pure BT (see Refs. [27–29]). Crucially, the rhombohedral–orthorhombic transition occurs at ~ 320 K (cooling) and ~ 345 K (heating). Thus, rhombohedral order remains stable above 300 K, with modest thermal hysteresis, which fulfills the crystallographic condition for our topological textures at room temperature.

The first attempts to induce nanodomains at 293 K started from a single-domain state, where we inverted the

polarization locally using a [111]-oriented cylindrical seed (as in the previous sections). Although domains formed and persisted for tens of picoseconds, they eventually relaxed back to the single-domain state owing to thermal fluctuations. Under these conditions, robust zero-field retention was not achieved. As a second attempt, and following the concept of Stepková and Hlinka [14], we applied a local electric field collinear with [111] to write and stabilize a reversed cylindrical domain. A local field of 350 kV/cm reliably produced and maintained nanodomains at 293 K, for larger diameters, 250 kV/cm was sufficient, though we used 350 kV/cm (a field in the near-saturation regime of our EH-MD protocol, for the P-E loop see Fig. S6 within the Supplemental Material [39]) consistently. Figures 4(b) and 4(c) show that domains persist throughout the simulation window as long as the field remains applied (volatile operation). Around the domain circumference, nontrivial topological textures emerge, closely resembling the low-temperature patterns but now carrying a plane-integrated charge of $Q = +4$ at 293 K. The internal structure exhibits fragmented local charge consistent with the fractionalized motifs described earlier. Although the stabilizing field is cylindrically defined, the resulting in-plane pattern reflects the underlying rhombohedral anisotropy of the BT-based host lattice: Polarization rotation and wall closure preferentially follow the symmetry-allowed (111) variants, yielding a threefold (3m) motif as a low-energy closure configuration [14]. Furthermore, along the nanodomain axis, the $-2/+4$ alternation is absent, instead the external field enforces a uniform $+4$ texture. In contrast, the random 12.5% BZT composition exhibits different behavior. Although a single-domain configuration can be prepared at 293 K in the supercell, introducing the local field destabilizes it and drives a transition to a multidomain state. Thermal fluctuations together with compositional disorder are sufficiently strong to destabilize single-domain retention under bias.

As for the interpretation, in the 12.5% superlattice at 293 K, a local field $E \parallel [111]$ can stabilize a single reversed cylinder, the wall adopts a nontrivial topological nature and every (111) projection yields $Q = +4$, indicating that $-\mathbf{E} \cdot \mathbf{P}$ overcomes thermal roughening and depolarizing costs while suppressing axial reversals. In contrast, in the 12.5% random composition, the same local field destabilizes a prepared single-domain and drives multidomain nucleation, showing that compositional disorder plus thermal fluctuations lower local nucleation barriers and favor multiple pinned walls under bias. Consequently, the random compositions do not sustain a single cylindrical domain or a uniform topological charge along z' under the writing field, whereas the ordered superlattice does. Thus, at room temperature, topology is field stabilized and volatile in the ordered case, but field-induced fragmentation dominates in the random composition, achieving robust retention in disordered samples will require raising wall stiffness and suppressing disorder-assisted nucleation, as discussed below.

Practically, this means room-temperature operation is field programmable and volatile: Domains can be written and held as long as the field is applied, and they relax when it is removed. Pathways to nonvolatile retention at 300 K include raising the domain-wall energy and suppressing thermal roughening through epitaxial strain (to stabilize the rhom-

bohedral state and increase anisotropy), employing strain gradients, electrostatic engineering, and periodic pinning (superlattices or patterned compositional modulation) to stabilize the nontrivial topological wall structure. These routes provide concrete directions for stabilizing topological textures at room temperature without a sustaining field.

IV. FINAL REMARKS AND SUMMARY

Using an EH framework benchmarked against DFT, we established that BZT supports a rich set of ferroelectric topological textures. In the 12.5% superlattice, chemical doubling along [111] yields an alternation of textures: one half hosts the canonical -2 antiskyrmion (six $-1/3$ topological quarks), the other a $+4$ skyrmion (six $+2/3$ topological quarks). Plane-resolved analyses show that the two chemical halves preserve the same six-vortex scaffold but exhibit distinct core-level polarization textures, yielding an integer offset of $+1$ per vortex in the slice charge, which is confirmed by difference maps of the local topological charge density. In random BZT, nanodomains remain inducible and stable at 1 K across 0–12.5% Zr, but disorder pins and distorts vortices, producing a skyrmion-glass-like state with spatially heterogeneous fractionalization and $Q(z')$ fluctuations. Thermal ramping reveals a nonmonotonic intrinsic T_{collapse} : it drops with initial Zr substitution (minimum near 6–8%) and partially recovers toward 12.5%, reflecting competition between average ferroelectric softening and disorder pinning/self-averaging. This trend was verified across three independent random-compositions realizations; however, because finite-size effects and stochastic disorder produce configuration-dependent scatter in T_{collapse} , the quantitative bounds are indicative only until tested with larger supercells and a broader ensemble. Finally, near room temperature, the 12.5% superlattice is rhombohedral (cooling ~ 320 K, heating ~ 345 K). Cylindrical nanodomains cannot be retained at 293 K without bias, but a local field (~ 350 kV/cm, $[111]$) writes and holds domains whose wall selects a nontrivial topological character, giving $Q = +4$ on every (111) projection (no $-2/+4$ alternation). In contrast, the 12.5% random composition does not retain a single domain under the same bias, instead the field nucleates multidomain states because of disorder-assisted instabilities.

The unit-cell doubling in the ordered system restructures the local anisotropy landscape, enabling the integer shift of plane-resolved charge without moving vortex cores. In random compositions, quenched anisotropy and random-field components pin and shear domain walls, enabling partial charge transfers and preventing a unique texture classification. With increasing Zr, T_{collapse} reflects the balance between reduced wall energy (softening) and disorder-induced pinning. At 293 K, line tension and depolarizing energy are insufficient for zero-field retention, but an external field stabilizes a nontrivial topological wall in the superlattice, whereas disorder in the composition lowers local nucleation barriers and drives fragmentation into a multidomain state.

This work establishes BZT as a practical platform for engineered ferroelectric topology, from fractionalized ($-1/3$, $+2/3$) topological quarks at 1 K to field-stabilized $Q = +4$ textures near room temperature. We also introduced an optional $\mathbb{Z}_2$ bookkeeping perspective, a compact

symmetry-based language for the chemically doubled motif, that captures the systematic integer (+1 per vortex) offset between chemically distinct regions. Microscopically, our data indicate that this offset is mediated by localized Bloch-point-like conversion events, enabled by Zr-assisted suppression of the polarization amplitude ($|p| \rightarrow 0$) at/near vortex axes within the interfacial region. What remains to be clarified is the detailed spatial and temporal statistics of these conversion events, how localized they remain as a function of temperature, disorder, and skyrmion diameter, and how the availability of multiple low- $|p|$ sites in broader cores affects the robustness of the alternation.

On the materials side, the proposed 12.5% ordered superlattice provides a clean phenomenology but may be difficult to synthesize with long-range chemical order across device-relevant areas. Fortunately, several alternative routes could possibly stabilize the rhombohedral phase near 300 K without strict chemical ordering: epitaxial biaxial strain [54] (via substrate choice and orientation), compositional tuning or gradients [27,35] (chemical pressure), and electrostatic engineering [55] (improved screening to suppress depolarizing fields). These approaches could also increase domain-wall energy and can enhance retention.

It is worth noting the broader potential of the topological textures discussed here and in the literature. If the internal fractional structure could be externally addressed and read out, topology would move beyond a binary scheme toward true multistate functionality. Instead of simply switching a nanodomain on or off, information could also be stored in its internal configuration, an appealing prospect for memory concepts as well as neuromorphic schemes. Realizing this remains a longer-term vision: experimental confirmation of such textures and strategies for their stabilization are the immediate priorities, with epitaxial

strain, chemical substitution, and related approaches offering promising routes.

In summary, BZT emerges as a versatile playground for ferroelectric topology, where both ordered and random chemistries support textures with rich fractional internal structure and clear thermal stability windows from cryogenic temperatures to near room temperature, including field-stabilized states at 293 K. These results identify strain, electrostatics, and compositional patterning as promising avenues for systematic studies of the creation, manipulation, and readout of topological textures, setting the stage for broader exploration.

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DATA AVAILABILITY

The data supporting the findings of this study are not publicly available but are available from the author upon reasonable request.

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