

Lattice Excitations with Finite Polarization and Magnetization

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Ferrons are a type of quasiparticle corresponding to elementary excitations of the ferroelectric order. Analogously to how magnons modulate and transport magnetization, ferrons modulate and transport electric polarization. Here, we introduce *multiferrons* as elementary excitations with both electric and magnetic character. Multiferrons lead to a tilt and elliptical precession of the polarization and at the same time create a magnetization through the mechanism of dynamical multiferroicity. Using first-principles calculations for LiNbO₃, we show that the electric polarization of multiferrons is perpendicular to the equilibrium ferroelectric polarization, whereas the magnetization is parallel to it. Our calculations further demonstrate that multiferrons carry net electric and magnetic quadrupole and octupole moments, which we term multipolons. These multipolons could couple to internal multipolar degrees of freedom, for example in altermagnets, or to external probes such as neutrons, leading to potentially experimentally observable phenomena following coherent or thermal excitation of multiferrons.

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Introduction—Quasiparticles are fundamental excitations of ordered electronic and structural phases in solids. A prototypical example are magnons, excitations of magnetic order that lead to spin precession and a change in magnetization or Néel vector along the equilibrium orientation [1,2]. Recently, ferrons have emerged analogously as fundamental excitations of ferroelectric order that carry a net polarization opposing the equilibrium ferroelectric polarization, as illustrated in Fig. 1(a) [3–11]. Ferrons can be described as electric dipole-carrying phonons existing in the intrinsically anharmonic potential energy landscape of ferroelectrics, leading to new forms of polarization transport and control [12].

Here, we introduce a new type of quasiparticle called the *multiferron*, a fundamental excitation of nonmagnetic ferroelectrics that carries both an electric polarization and a magnetization. Multiferrons can be described as elliptically polarized in-plane ferrons that carry a net polarization perpendicular to the equilibrium ferroelectric polarization [Fig. 1(b)] and carry a magnetization parallel to it [Fig. 1(c)].

This leads to a tilt and precession of the total electric polarization in the system. We perform first-principles calculations for multiferrons in the prototypical ferroelectric lithium niobate (LiNbO₃), for which we compute the quantized polarization and magnetization, as well as the dynamical response to the coherent excitation by an ultra-short terahertz pulse. We find that in addition to net electric polarization and magnetization, multiferrons also carry net quadrupole and octupole moments. These results open a pathway to controlling and transporting electric and magnetic dipole and multipole properties.

Multiferrons—We begin by calculating the finite electric polarization and magnetization that give rise to multiferrons. LiNbO₃ is a ferroelectric semiconductor crystallizing in the rhombohedral *R3c* space group [13] that exhibits an optical band gap of 3.7 eV [14]. Its primitive unit cell consists of ten atoms, resulting in 30 phonon modes characterized by the irreducible representations *A*₁, *A*₂, and *E*. We determine the structural and electronic properties of LiNbO₃ using density functional theory, the details of which can be found in Note 1 in Supplemental Material (SM) [15] (see also Refs. [16–37] therein).

Electric polarization: We model the ferroelectric polarization *P* of LiNbO₃ by a double-well potential [Fig. 1(a)] in the Landau-Devonshire theory as

$$V(P) = \alpha P^2 + \beta P^4 + \gamma P^6, \quad (1)$$

with $\alpha < 0$ and $\beta, \gamma > 0$, yielding minima at the equilibrium ferroelectric polarization of $P_0 = \pm 79.9 \mu\text{C}/\text{cm}^2$. Owing to the intrinsic anharmonicity at these minima,

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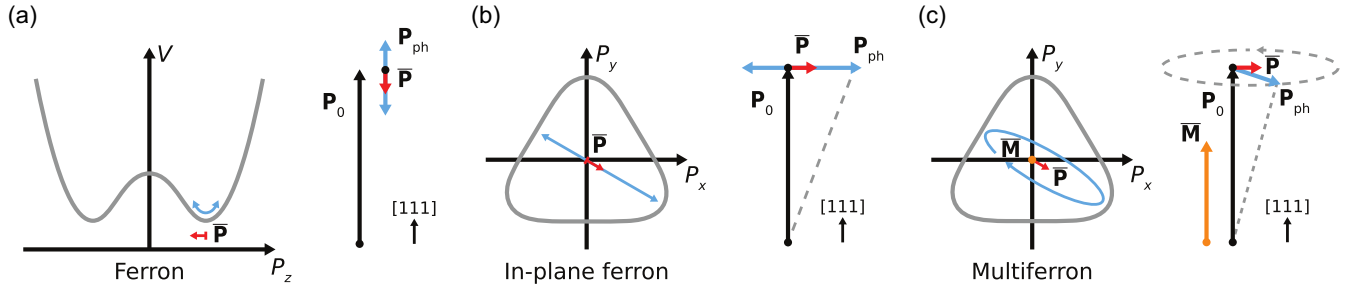


FIG. 1. Ferrons in LiNbO₃. (a) Excitation of A_1 modes leads to anharmonic oscillations of the electric polarization $\mathbf{P}_{ph}$, generating ferrons with a net polarization $\bar{\mathbf{P}}$, reducing the magnitude of the ferroelectric polarization $\mathbf{P}_0$. (b) Linear excitation of anharmonic E modes produces in-plane ferrons with a net polarization perpendicular to the ferroelectric polarization, $\bar{\mathbf{P}} \perp \mathbf{P}_0$, leading to a tilting and increase of the total polarization (dashed line). (c) Elliptical excitation of anharmonic E modes yields multiferrons, in which the total polarization precesses, leading to a net in-plane polarization and a net out-of-plane magnetization $\bar{\mathbf{M}}$. Polarization dynamics are shown in blue, net ferron polarization in red, and magnetization in orange.

excitations along the polarization coordinate carry a net polarization and are therefore referred to as ferrons [3]. These excitations can be decomposed into the infrared-active (IR-active) A_1 modes, with the biggest contribution coming from the low-frequency mode at 7.16 THz [38,39] (SM, Note 1 [15]). We therefore express the polarization in terms of the phonon amplitude Q as

$$\mathbf{P}_{ph} = \mathbf{Z}Q/V_c, \quad (2)$$

where V_c is the unit cell volume, and $\mathbf{Z} = \sum_n \mathbf{Z}_n^* (\mathbf{q}_n / \sqrt{\mathcal{M}_n})$ is the mode effective charge given by the Born effective charge tensor $\mathbf{Z}_n^*$, the phonon eigenvector $\mathbf{q}_n$, and the mass $\mathcal{M}_n$ of atom n . Substituting Eq. (2) into Eq. (1) yields an equivalent double-well potential in terms of Q , which provides a natural starting point for analyzing lattice excitations in LiNbO₃. In the following, we will derive the net electric polarization and magnetization generated by multiferrons.

Close to the minima at $\pm P_0$, the potential energy of a mode can be described using a reduced potential energy expression with the form

$$V(Q) = \frac{\omega^2}{2} Q^2 + aQ^3, \quad (3)$$

with phonon amplitude Q , angular frequency ω , and anharmonicity a . This one-dimensional potential applies to the A_1 modes, as well as to the E modes along the high-symmetry directions (SM, Note 2 [15]). The cubic term acts as a self-rectification of the mode, for which we obtain a net phonon displacement $\bar{Q} = -(3a/\omega^2) \langle Q^2 \rangle$, leading to a net polarization given by

$$\bar{\mathbf{P}} = -\frac{\mathbf{Z}}{V_c} \frac{3a}{\omega^2} \langle Q^2 \rangle, \quad (4)$$

where $\langle Q^2 \rangle = \hbar/\omega$ is the mean-squared amplitude of a single phonon. The polarization associated with a single

phonon per unit cell, obtained for linear excitations of the A_1 and E modes using Eq. (4), is summarized in SM, Note 3 [15]. Excitations of the A_1 modes decrease the magnitude of the total polarization [Fig. 1(a)], whereas excitations of the E modes lead to an increase and tilting of the total polarization [Fig. 1(b)], which could be referred to as Higgs-like and Goldstone-like ferrons, respectively [5].

Magnetization: When the degenerate E modes are excited circularly, the resulting ionic motion follows circular or elliptical trajectories. Such motion results in a temporally rotating electric polarization $\mathbf{P}_{ph}$, which gives rise to an out-of-plane net magnetization $\bar{\mathbf{M}}$ via the mechanism of dynamical multiferroicity [40,41] [Fig. 1(c)], as given by

$$\bar{\mathbf{M}} \propto \mathbf{P}_{ph} \times \partial_t \mathbf{P}_{ph}. \quad (5)$$

Microscopically, the effect originates from atomistic electromagnetic loops created by the circular motion of the ions, which give rise to phonon modes carrying a net magnetization, even in nonmagnetic materials [40–55]. In experiment, the mechanism has been confirmed to generate giant effective magnetic fields corresponding to this magnetization [56–59]. For a pair of degenerate modes, α and β , the magnetization associated with a single circularly polarized phonon per unit cell can be written as $\bar{\mathbf{M}} = (\hbar/V_c) \sum_n [e\mathbf{Z}_n^* / 2\mathcal{M}_n] (\mathbf{q}_{\alpha,n} \times \mathbf{q}_{\beta,n})$, where e is the elementary charge, and $\mathbf{q}_{\alpha,n}$ and $\mathbf{q}_{\beta,n}$ are the normalized mode eigenvectors of atom n in modes α and β . The resulting magnetization values $|\bar{\mathbf{M}}|$ for a single circularly polarized phonon are provided in SM, Note 3 [15].

In addition to the out-of-plane magnetization arising from the circular or elliptical excitation of degenerate modes, the rotating polarization $\mathbf{P}_{ph}$ also contains a component perpendicular to the ferroelectric polarization of the material $\mathbf{P}_0$, which produces a radial magnetization component given by

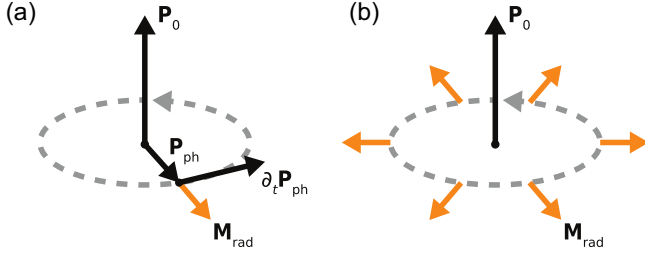


FIG. 2. Magnetization induced by circular and elliptical excitation of the E modes in LiNbO_3 . (a) Superposition between the static ferroelectric polarization $\mathbf{P}_0$ and rotating phonon polarization $\partial_t \mathbf{P}_{ph}$. (b) Resulting radial magnetization $\mathbf{M}_{rad}$.

$$\mathbf{M}_{rad} \propto \mathbf{P}_0 \times \partial_t \mathbf{P}_{ph}. \quad (6)$$

$\mathbf{M}_{rad}$ is perpendicular to both $\mathbf{P}_0$ and the time derivative of $\mathbf{P}_{ph}$, as shown in Fig. 2. Because the out-of-plane magnetization and radial magnetization both scale with the magnitude of the ionic charge current, the contribution of each atom to the radial magnetization can be expressed as

$$|\mathbf{M}_{rad,n}| = |\bar{\mathbf{M}}_n| \frac{|\mathbf{P}_0|}{|\mathbf{P}_{ph,n}|}, \quad (7)$$

where $|\mathbf{P}_{ph,n}|$ and $|\bar{\mathbf{M}}_n|$ denote the atomic contributions to the phonon-induced polarization and magnetization, respectively. The radial magnetization is then obtained by summing over all atomic contributions, $\mathbf{M}_{rad} = \sum_n |\mathbf{M}_{rad,n}| \hat{\mathbf{M}}_{rad,n}$, where $\hat{\mathbf{M}}_{rad,n}$ is the unit vector indicating the direction of each atomic contribution.

Interestingly, elliptical excitations of E modes produce both a net polarization and magnetization [Fig. 1(c)]. Their elliptical trajectories generate a net out-of-plane magnetization $\bar{\mathbf{M}}$, while simultaneously probing the anharmonicity of the potential landscape, which produces a net in-plane polarization $\bar{\mathbf{P}}$. We accordingly term these excitations *multiferrons*.

Coherent multiferrons—To study the polarization and magnetization dynamics of multiferrons, we numerically solve the equations of motion for the modes $\alpha \in \{a, b\}$

$$\ddot{Q}_\alpha + \kappa_\alpha \dot{Q}_\alpha + \partial_{Q_\alpha} V = \mathbf{Z}_\alpha \cdot \mathbf{E}, \quad (8)$$

where $\kappa_\alpha = \omega_\alpha / (20 \cdot 2\pi)$ is the experimental phonon linewidth [27], and V the anharmonic potential energy. For two degenerate E modes, the potential energy can be written as

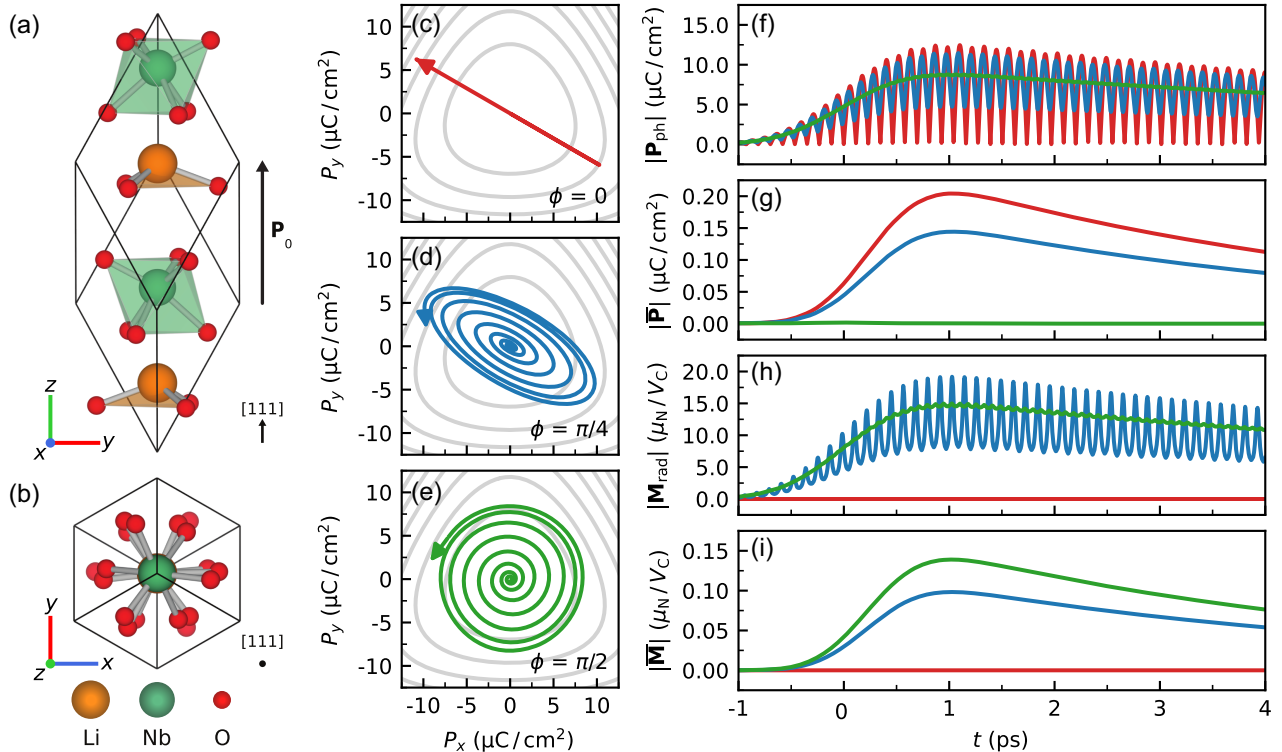


FIG. 3. Electric polarization and magnetization dynamics induced by resonant excitation of degenerate E modes at 4.32 THz in LiNbO_3 . (a),(b) Side and top views of the unit cell of LiNbO_3 . (c)–(e) Polarization dynamics driven by linearly ($\phi = 0$), elliptically ($\phi = \pi/4$), and circularly ($\phi = \pi/2$) polarized pulses in the time window from -1.0 to 0.5 ps. Equipotential lines representing the symmetry of the polarization are shown in gray. (f),(g) Time evolution of the radial polarization $|\mathbf{P}_{ph}|$ and net polarization $|\bar{\mathbf{P}}|$. (h),(i) Corresponding time evolution of the radial magnetization $|\mathbf{M}_{rad}|$ and net magnetization $|\bar{\mathbf{M}}|$.

$$V(Q_a, Q_b) = \frac{\omega_a^2}{2} Q_a^2 + \frac{\omega_b^2}{2} Q_b^2 + a_1 Q_a^3 + a_2 Q_a^2 Q_b + a_3 Q_a Q_b^2 + a_4 Q_b^3, \quad (9)$$

where $\omega_a = \omega_b \equiv \omega$ and a_i ($i = 1, \dots, 4$) are the anharmonic coupling coefficients. The right-hand side of Eq. (8) describes the external driving force from a laser pulse, where $\mathbf{Z}_\alpha$ is the mode effective charge that determines the coupling to the electric field $\mathbf{E}$. The temporal profile and polarization of the driving field govern the amplitude and phase of the coherent phonon response. The functional form used to model the laser pulse is given in SM, Note 4 [15].

In Fig. 3, we present the dynamics of the degenerate E modes at 4.32 THz in LiNbO₃, with other E modes shown in SM, Note 5 [15]. Figures 3(a) and 3(b) show the unit cell from two different crystallographic directions, where the E modes are polarized in the xy plane. To demonstrate the multiferroic dynamics, we excite the low-frequency modes using linear, elliptical, and circular laser pulses, along the high-symmetry lines of the potential energy surface, as shown in Figs. 3(c)–3(e). In all cases, the polarization dynamics follow the polarization of the laser pulse: a linearly polarized pulse leads to linear oscillations of the polarization, whereas elliptically and circularly polarized pulses generate a precessing polarization. This behavior is also reflected by the time evolution of the magnitude of radial polarization $|\mathbf{P}_{\text{ph}}|$ in Fig. 3(f).

We next investigate how the phonon anharmonicity leads to a net polarization $|\tilde{\mathbf{P}}|$ upon driving the E modes, which we show in Fig. 3(g). For both linear and elliptical excitations, a nonzero in-plane polarization is generated that tilts the overall polarization of the material. The envelope of the net polarization follows the time-dependent phonon population number, $|\tilde{\mathbf{P}}| \propto \langle Q^2 \rangle \propto N$, which decays on a timescale determined by the phonon linewidth κ_α . $|\tilde{\mathbf{P}}|$ is largest for linearly polarized driving and reduced by a factor of $\sqrt{2}$ for elliptically polarized driving. Circular excitations probe the anharmonic potential energy surface uniformly and do not create net polarization.

Upon investigating magnetization dynamics, we observe a substantial radial magnetization $|\mathbf{M}_{\text{rad}}|$ for elliptical and circular excitation, which we show in Fig. 3(h). This effect originates from the superposition of the rotating polarization and the ferroelectric polarization, as described by Eq. (6). Similarly, the net out-of-plane magnetization $|\tilde{\mathbf{M}}|$ is only produced by elliptical and circular excitations [Fig. 3(i)]. The envelope of $|\tilde{\mathbf{M}}|$ follows the time-dependent phonon population in the same way as $|\tilde{\mathbf{P}}|$. Notably, the magnitude of the radial magnetization is two orders of magnitude larger than that of the net out-of-plane magnetization.

Elliptically polarized driving yields both a net in-plane polarization and a net out-of-plane magnetization as a result of the coherent excitation of multiferroics. The relative

strength of the induced electric polarization and magnetization can be tuned continuously by tuning the ellipticity of the laser pulse, as shown in SM, Note 5 [15]. The multiferroics further generate a rotating radial magnetization and polarization parallel to each other (Fig. 2). We will show in the following that these rotating contributions additionally lead to the emergence of electric and magnetic multipole moments.

Multipolons—We next investigate the multipolar nature of the radial polarization and magnetization induced by the multiferroics, which we express using quadrupole tensors Q_{ij} . Within each unit cell, the contributions of the atoms to the quadrupole tensors are given by

$$\langle Q_{n,ij}^P \rangle = \langle u_{n,i} P_{\text{ph},n,j} \rangle - \frac{1}{3} \delta_{ij} \sum_k \langle u_{n,k} P_{\text{ph},n,k} \rangle, \quad (10)$$

$$\langle Q_{n,ij}^M \rangle = \langle u_{n,i} M_{\text{rad},n,j} \rangle - \frac{1}{3} \delta_{ij} \sum_k \langle u_{n,k} M_{\text{rad},n,k} \rangle, \quad (11)$$

where $\langle \dots \rangle$ denotes an average over the phonon period, $i, j, k \in \{x, y, z\}$ indicate the Cartesian components of the vectors, $u_{n,i} = \sum_\alpha Q_\alpha (q_{\alpha,n,i} / \sqrt{M_n})$ are the atomic displacements, and δ_{ij} is the Kronecker delta function. Each total quadrupole tensor component is obtained by summing over all atomic contributions: $\langle Q_{ij} \rangle = \sum_n \langle Q_{n,ij} \rangle$. In a similar manner, the octupole tensor can be computed, a description of which is provided in SM, Note 6 [15]. These multipolar tensors are constructed as sums over the individual contributions from the local atomic displacements.

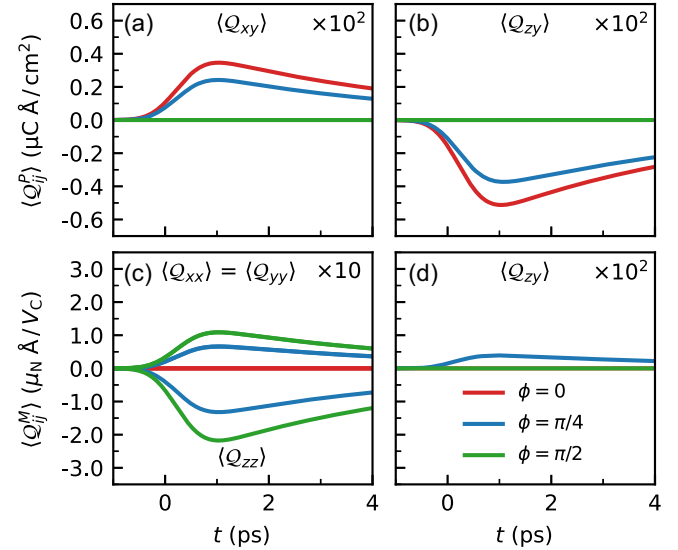


FIG. 4. Time-averaged quadrupole tensors of radial polarization (top) and magnetization (bottom) for linearly ($\phi = 0$), elliptically ($\phi = \pi/4$), and circularly ($\phi = \pi/2$) polarized pulses. (a), (b) Off-diagonal quadrupole tensor contributions to radial polarization $\mathbf{P}_{\text{ph}}$. (c), (d) Diagonal and off-diagonal quadrupole tensor contributions to radial magnetization $\mathbf{M}_{\text{rad}}$.

Figure 4 shows the temporal evolution of cycle-averaged components of the polarization and magnetic quadrupole tensors upon excitation by linearly, elliptically, and circularly polarized laser pulses. A complete overview of all components is provided in SM, Note 6 [15]. Notably, the nonzero $\langle Q_{xy} \rangle$ component in Fig. 4(a) can be used to describe the breaking of the axial symmetry of the radial polarization $\mathbf{P}_{\text{ph}}$ for both linear and elliptical excitations. Additionally, the finite value of $\langle Q_{zy} \rangle \neq 0$ [Fig. 4(b)] indicates that such excitations also lead to a small out-of-plane tilt of the polarization.

Focusing on the multipole moments of the radial magnetization $\mathbf{M}_{\text{rad}}$, we observe that circular and elliptical excitations also yield substantial nonzero diagonal components to the quadrupole tensor, i.e., $\langle Q_{ij}^M \rangle \neq 0$ [Fig. 4(c)]. Linear excitations do not yield any diagonal components since they do not give rise to any radial magnetization. Notably, elliptical excitations also give rise to a nonzero zy component in the quadrupole tensor as seen in Fig. 4(d). This off-diagonal term tilts the magnetization distribution out of the transverse plane, breaking the in-plane symmetry that is present for circular excitations.

Our results show that multiferrons can generate structured polarization and magnetization patterns with multipole moments. The induced finite quadrupole and octupole tensor components can be tuned by changing the ellipticity of the incident laser pulse, similar to the net polarization and magnetization components. We therefore term these excitations *multipolons*.

Discussion—We have performed our calculations for the example of LiNbO_3 , however, multiferrons and multipolons can be created in all ferroelectric materials hosting doubly degenerate optical phonons. The size of the magnetic moment associated with multiferrons depends on the effective charges of the ions, making oxide perovskites [41,57] or other materials with large phonon magnetic moments such as $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ [46,47] attractive candidates for large multiferronic effects. As the multipolar moments are proportional to the ferroelectric polarization, oxide perovskites are also a promising choice to observe multipolons.

While multiferrons share similarities with magnetoferons and electromagnons, which are hybrid quasiparticles that appear in multiferroic materials [60], they differ in two aspects. First, multiferrons do not require magnetic order to be present. Second, multiferrons carry both a finite polarization and magnetization, whereas the other quasiparticles carry either only one (magnetoferons) or neither (electromagnons and circularly polarized phonons). In contrast, multiferrons do not require magnetic order to be present. Furthermore, recent predictions show that nonlinear phonon interaction allows for electric polarization and magnetization to be created simultaneously in nonpolar nonmagnetic materials [54]. These materials do not host multiferron quasiparticles however, as their symmetry does not allow for Q^3 -type anharmonicities.

Coherent excitation of multiferrons with an ultrashort laser pulse simultaneously generates macroscopic electric polarization and magnetization and provides a path to controlling multiple ferroic orders at once. In addition, the multipolar character of multiferrons opens possibilities regarding their coupling to external magnetic systems, as magnetic multipolar order plays an important role in orbital magnetism [61] and altermagnetism [62], and has recently been shown to couple to lattice vibrations [63,64]. The magnetic multipoles could be detected directly using inelastic neutron scattering, where signals can be attributed directly to magnetic quadrupoles [65].

While the coherent excitation of multiferrons with light demonstrated here occurs at the Brillouin-zone center, multiferrons at finite wave vectors can be excited thermally. In ferroelectric materials, IR-active phonon branches carry nonzero angular momentum and magnetic moments [66]. Although polar modes are generally considered in the limit $\mathbf{q} = 0$, transport experiments have shown that ferrons have substantial group velocity [8,9]. Therefore, the pyrocaloric effects which arise from ferrons [3] can be expected to have magnetocaloric complements in multiferrons. A thermal magnetization from multiferrons, like the thermally induced polarization from ferrons, would arise from broken rotational symmetry in the anharmonic potential at $\mathbf{q} \neq 0$. As propagating ferrons can transmit signals over micrometer distances [8,9], they may find potential applications in information technology. Ferron transport can be created by electric fields and temperature gradients [67], whereas multiferrons could further couple to magnetic fields, opening new possibilities for creating and manipulating their transport. To understand the transport properties of multiferrons, further study of their behavior at finite wave vectors is therefore required.

During the preparation of this manuscript, we became aware of a closely related study on multiferrons that was recently posted online [68].

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Data availability—The data that support the findings of this article are openly available [69].

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