Introducing artificial strain in epitaxial thin films is an effective strategy to alter electronic structures of transition metal oxides (TMOs) and to induce novel phenomena and functionalities not realized in bulk crystals. This study reports a breaking of the conventional trade-off relation in thermopower ($S$)–conductivity ($\sigma$) and demonstrates a 2 orders of magnitude enhancement of power factor (PF) in compressively strained LaTiO$_3$ (LTO) films. By varying substrates and reducing film thickness down to 4 nm, the out-of-plane to the in-plane lattice parameter ratio is controlled from 0.992 (tensile strain) to 1.034 (compressive strain). This tuning induces the electronic structure change from a Mott insulator to a metal and leads to a 10$^3$-fold increase in $\sigma$ up to 2920 S cm$^{-1}$. Concomitantly, the sign of $S$ inverts from positive to negative, and both $\sigma$ and $S$ increase and break the trade-off relation between them in the n-type region. As a result, the PF ($=S^2\sigma$) is significantly enhanced to 300 $\mu$W m$^{-1}$K$^{-2}$, which is 10$^4$ times larger than that of bulk LTO. Present results propose epitaxial strain as a means to finely tune strongly correlated TMOs close to their Mott transition, and thus to harness the hidden large thermoelectric PF.

1. Introduction

Since the discovery of large thermopower ($S$) accompanied by high electrical conductivities ($\sigma$) in strongly correlated transition metal oxides (TMOs), such as Na$_x$CoO$_2$,[1] the interplay of thermoelectricity and electronic correlations has been recognized as a potential source for high-performance thermoelectrics.[2–5] Indeed, the coexistence of large $S$ and high $\sigma$ causes a large power factor (PF = $S^2\sigma$).[6] Therefore, strongly correlated TMOs continue to be explored for their thermoelectric properties.

An established way to control the thermoelectric properties of TMOs is carrier doping through the addition of impurity elements, which has led to high PFs in La-doped SrTiO$_3$,[7] rare-earth-doped CaMnO$_3$,[8] and Sr-doped LaCoO$_3$.[9] However, the enhancement of PF is restricted by the well-known trade-off relationship.
between σ and S.\(^{16,10}\) Both σ and S depend on carrier concentration n but possess opposite relations based on the carrier-diffusion model; σ increases with growing n whereas S decreases, limiting the maximum PF at a certain n. Thus we can expect decoupling this trade-off beyond the carrier-diffusion model will further improve the thermoelectric performance of TMOs.

Here, we discovered an unusually large PF enhancement by breaking the trade-off relation between σ and S in a lattice-strain controlled TMO of LaTiO\(_3\) (LTO). Introducing artificial strain in epitaxial thin film has been an effective strategy to alter electronic structures of TMOs and has shown to manipulate various physical properties of TMOs, such as metal–insulator transitions,\(^{11,12}\) superconducting properties,\(^{13,14}\) and magnetic properties.\(^{15,16,17}\) The effect of epitaxial strain on thermoelectric properties is systematically controlled from -0.36% (tensile strain) to 1.70% (compressive strain) and varies approximately linearly with c/a. The out-of-plane ε\(_{zz}\) has the opposite sign and reaches up to 1.69% under in-plane compression. Notably, however, ε\(_{xx}\) becomes virtually constant for LTO films with t thinner than 10 nm on LaAlO\(_3\) substrate (i.e., c/a > 1.03). These strains translate into Poisson ratios ν = ε\(_{xx}\)/ε\(_{yy}\) ≥ 0.4 for the films with c/a < 1.03, but that drastically shrinks with t to reach ν ≈ 0.33 for the thinnest LTO film on LaAlO\(_3\) substrate (inset to Figure 1e). The consequences for the perovskite unit cell volume V are shown in Figure 1e. Consistent with ν < ½, LTO thin films are not volume-conserving and V shrinks with growing c/a. Following the sharper decreases in the Poisson ratio at larger c/a, the volume compression accelerates for thinner films. In this work, we exploit the enhanced compressibility of LTO thin films on LaAlO\(_3\) substrate to generate larger structural anisotropies c/a.

Besides tuning c/a and V, epitaxial strain may lead to atomic relaxations that lie outside the restrictions of the bulk space group. For a better understanding, we calculated total energetics of LTO for different symmetries from first principles, using density functional theory (DFT) (for details see the Experimental Section).

**Figure 2** displays the total energy as a function of the in-plane lattice parameter a, where c axis length and internal coordinates were relaxed so as to take minimum total energy. We identify two phases that are predicted to be more stable than the bulk structure Pbnm, i.e., I4/mcm with the rotational pattern a\(^b\) a\(^c\) c\(^b\) (in the Glazer notation) for compressive strain and I\(_{1m}ma\) with a\(^b\) b\(^c\) c\(^a\) for tensile strain. At equilibrium lattice parameters (the dashed lines at total energy minima for I4/mcm at a = 3.93 Å and for I\(_{1m}ma\) at a = 3.98 Å in Figure 2a), the calculated c/a agrees satisfactorily with the experimental data within a 1% error (Figure 2b). The predicted stable structures are depicted in Figures 2c,d. While octahedral distortions are negligible (all Ti–O distances ≈ 2.0 Å), epitaxial strain causes the Ti–O\(_3\) octahedra to rotate in the a-b (out...
of a-b) plane in the I4/mcm (Imma) phase, with the in-plane and the out-of-plane Ti–O–Ti angles of 157° and 156°, respectively.

Next, we discuss how these strain-induced crystallographic changes modify the electronic structure, focusing on the bandwidth (kinetic energy), the anisotropy (effective dimensionality), and crystal fields (degeneracies). Figure 2e,f shows the Ti 3d-orbital splitting,[23] resulting in a charge-transfer from d\(_{xy}\) to d\(_{zz}\) (d\(_{xy}\) orbital is lowest in energy, as found for bulk LTO).[22] Importantly, compressive strain tunes and, eventually, inverts this t\(_{2g}\) orbital splitting,[23] resulting in a charge-transfer from d\(_{xy}\) to the (at 300 K quasidegenerate) d\(_{x^2-y^2}\) and d\(_{yz}\) orbitals. Crystallographic details notwithstanding, the qualitative effect of strain onto hoppings and crystal fields is hence stable irrespective of the realized space-group under strain, see also Ref. [23].

Figure 3a,b shows the c/a dependence of a) \(\sigma\) and b) \(S\) at room temperature (RT) for the LTO films on different substrates (open symbols) and those with varying \(t\) on LaAlO\(_3\) substrates (closed red circles). With growing c/a, \(\sigma\) drastically increases from 2.2 S cm\(^{-1}\) (c/a = 0.993, tensile strain), which is close to the bulk value 3 S cm\(^{-1}\) (the black hexagons)[20], up to notable 60 S cm\(^{-1}\) (c/a = 1.034, compressive strain). The S of bulk LTO is positive with \(S_{\text{bulk}} = +60\ \mu\text{V K}^{-1}\).[10] Also LTO films with small c/a have positive \(S\), but its magnitude shrinks for increasing c/a.
Figure 2. Epitaxial strain dependences of DFT total energy and electronic structure of LTO through varying the in-plane lattice parameter $a$. a) Calculated total energy ($E$) of LTO for tetragonal $I4/mcm$ (octahedral rotation $a^0 a^0 c^-$ in Glazer’s notation), and orthorhombic $Imma$ ($a^- b^0 b^0$), $Pnma$ ($a^- b^- b^-$) structures. b) Calculated $c/a$ values at the equilibrium $a$ values (the red squares and the $E$ minima indicated by the dashed lines in (a)). Experimental data are shown for comparison (the gray circles and diamonds). c,d) Relaxed crystal structures of $I4/mcm$ c) and $Imma$ d). e) Strain dependence of Ti 3d nearest-neighbor hopping parameters, $|t_{ij}|$. f) Strain dependence of the on-site energy difference (crystal-field) $\Delta E$ for $d_{xy}$, $d_{xz}$, and $d_{yz}$ orbitals with respect to the orbital average energy $(E_{d_{xy}} + E_{d_{xz}} + E_{d_{yz}})/3$ for $I4/mcm$ (open) and $Imma$ (closed symbols).

At a critical value $c/a \approx 1.028$, $S$ eventually changes its sign and reaches $-40$ $\mu$V K$^{-1}$ for the thinnest LTO film on LaAlO$_3$. LTO films on YAlO$_3$ and LSAT with $|\Delta a/a| > 1\%$, qualitatively display the same $S$ sign change (Figure S12, Supporting Information). For substrates with smaller $|\Delta a/a| < 1\%$, however, $S$ and $c/a$ are independent of $t$. We thus identify the $c/a$ ratio as a direct control parameter of the $S$ in strained LTO.

Figure 3c displays the $c/a$ dependence of $PF = S^2 \sigma$: With increasing $c/a$ up to $\approx 1.02$, PF grows moderately because $\sigma$ increases. Beyond the carrier polarity change at $c/a = 1.028$, PF is enhanced up to $300$ $\mu$W m$^{-1}$K$^{-2}$, which is $>10^2$ times larger than 1 $\mu$W m$^{-1}$K$^{-2}$ of LTO bulk. This spectacular boost in PF owes to the simultaneous increase of $\sigma$ and $S$ in the n-type region, which defies common wisdom. Usually, the optimization of PF follows a trade-off relation between $\sigma$ and $S$. Indeed, $\sigma$ is larger in metals while $S$ is larger in insulators due to the opposing tendency with carrier concentration. This trade-off relation between $\sigma$ and $S$ usually only allows PF optimizations to reach local maxima.
Here, in the compressively strained LTO films with \( c/a > 1.028 \) in the n-type region, the behaviors of \( \sigma \) and \( S \) are apparently decoupled, and PF can be enlarged globally.

Figure 4a shows the temperature (\( T \)) dependence of \( S \) for the p-type LTO film (\( c/a = 0.992 \)), tensile strain, indicated by the vertical arrow on the left side of Figure 3b) and the n-type LTO film (\( c/a = 1.034 \), compressive strain, indicated by the vertical arrow on the right side of Figure 3b). The \( T \) variations of \( |S| \) show opposite trends, i.e., \(|S| \) decreases with increasing \( T \) for the p-type LTO film, while increases with increasing \( T \) for the n-type one. As known from the Boltzmann transport theory based on the carrier-diffusion model, the electronic contribution of \( S \) in non-degenerated semiconductors is expressed as

\[
S = \frac{k_B}{e} \left( \frac{2}{3} \frac{m^*}{m_c} + A \right),
\]

where \( k_B \) is the Boltzmann constant, \( e \) is the elementary electric charge, \( E_c \) is the conduction band edge energy, and \( A \) is a transport constant that depends on the dominant scattering mechanism. While, \( S \) for metals or degenerate semiconductors is basically expressed as

\[
S = \frac{e^2}{4 \pi^2 \hbar^2} \left( \frac{2}{3} \frac{m^*}{m_c} \right) E_c (\text{Mott’s equation}).\]

The above results indicate the p-type LTO film corresponds to the semiconducting \( T \) dependence, which is consistent with that \( E_F \) locates in the Mott gap for bulk LTO. On the other hand, the n-type LTO film corresponds to a metallic \( T \) dependence, suggesting that the Mott gap is closed in the n-type LTO film. Note that we can find a small \( S \) peak at \( T = 25 \) K in the \( S-T \) curve of the n-type LTO film, which should originate from the phonon-drag effect.

Figure 4b–d shows \( T \) variations of carrier transport properties. Since it was difficult to measure reliable Hall voltages for all the LTO films presumably due to high carrier concentrations (i.e., small Hall voltage) and low carrier mobility, we estimate the weighted mobility (\( \mu_w \)) using the equation

\[
\mu_w = \frac{\ln(e)\pi^2 k_B^2}{8 e (2 m^* k_B T)^{3/2}} \left[ \frac{2 e^2}{2 m^* k_B T} + \frac{2 e^2}{2 m^* k_B T} \exp\left( \frac{2 e^2}{2 m^* k_B T} \right) \right],
\]

where \( h \) is Planck constant and \( m^* \) is the free electron mass. The \( \mu_w \) is related to the drift mobility \( \mu \) by \( \mu_w \approx \mu \left( \frac{n_e}{m^*} \right)^{1/2} \), where \( n_e \) is the density of states effective mass. The corresponding carrier density \( n_e \) is calculated by \( n_e = \sigma(\rho(\mu_w)) \). Although the \( T \) dependences of resistivity (\( \rho \)) for both the p-type and the n-type LTO films show similar semiconducting behaviors as seen in Figure 4b, this is an apparently wrong conclusion. Indeed, although \( \mu_w \) shows a similar trend with \( T \) for the p-type and the n-type LTO films (Figure 4c), \( n_e \) shows opposite \( T \) dependences (Figure 4d). The Arrhenius plot of \( n_e \) (i.e., \( \log \frac{n_e}{1000/\rho(T)} \)) shows a good straight line with the activation energy of 63 meV for the p-type LTO film, further supporting the conclusion that the p-type LTO film is a semiconductor with a finite Mott gap. On the other hand, the \( T \) dependence of \( n_e \) is small for the n-type one, being consistent with the above conclusion that the n-type LTO has a metallic electronic structure.

Here, we discuss why the electronic structure of LTO film changes from the Mott insulator state to the metallic state by compressive strain. The mechanism for Mott-insulating bulk LTO is explained by a combination of small bandwidths and reduced charge fluctuations through a Ti 3d \( t_{2g} \) orbital splitting, where the \( d_{yz} \) orbital has the lowest energy.\[12\] Our first-principles calculation results in Figure 2f demonstrated that compressive strain (growing \( c/a \) increases bandwidths, while also allowing for more charge fluctuations by doubling the degeneracy of the lowest \( t_{2g} \) orbital, where the \( d_{xy} \) and \( d_{xz} \) orbitals have the lowest energy. Figure 4e schematically depicts the electronic structures of the p-type LTO and the n-type LTO with Ti 3d electronic configuration based on these results. For the p-type LTO, \( E_F \) locates near the midgap energy between the lower and the upper Hubbard.
bands of the $d_{xz}$, $d_{yz}$ orbitals, where the $E_F$ slightly shifts to the lower Hubbard band and leads to the p-type semiconductor behavior. On the other hand, for the n-type LTO, it has a metallic electronic structure, where the one d electron occupies a hybridized band of $d_{x^2}$ and $d_{y^2}$ character, and thus it shows n-type conduction.

Next, we discuss the origin of the breaking of the trade-off relation. Figure 5a summarizes the relationship between $S$ and $\sigma$ for all the LTO films at RT. In the p-type region, the $S$ linearly decreases as a function of $\log \sigma$ with a slope of $-50 \mu V K^{-1}$ decade$^{-1}$ and passes through zero, resulting in the carrier polarity change from p-type to n-type. On the other hand, the unusual simultaneous increase in $|S|$ and $\sigma$ is observed in the highly conductive n-type region, which cannot be explained by the carrier-diffusion model. However, this relation should be reinterpreted in term of carrier density $n_w$, similar to Figure 4b–d. As mixed carrier conduction (i.e., electrons and holes contribute to electronic conducton) is expected in the vicinity of the p–n transition, $\mu_w$ and $n_w$ values were calculated with the data apart from the p–n transition. As shown in Figure 5b, $\mu_w$ largely increases with increasing $\sigma$, and farther larger $\mu_w$ are observed in the n-type region compared to those in the p-type region, which is similar to perovskite oxides where $\mu_w$ is larger in n-type region. Therefore, we can reinterpret the $S$–$\sigma$ relation in Figure 5a by the $S$–$n_w$ plots in Figure 5c, which reproduces usual $S$–$n$ relations known as Jonker plot, where $S$ decreases with increasing $n_w$, in both the p-type and the n-type regions.

Finally, we can conclude that, in the n-type region, both $S$ and $\sigma$ increase simultaneously with increasing $c/a$ ratio, which breaks the trade-off relation of the carrier-diffusion model, because $S$ is increased by the reduced $n_w$, as described in the carrier-diffusion model, while $\sigma$ is also increased by the enhancement of $\mu_w$ that surpasses the reduction in $n_w$. Note that the simultaneous increase in $S$ and $\sigma$ is previously reported in (Sr$_{0.85}$La$_{0.15}$)TiO$_3$–x films, where the oxygen vacancy formation increases $\sigma$, while $S$ is also increased due to the polaron mass enhancement.

3. Conclusion

In summary, we studied the thermoelectric response of LTO thin films by varying their electronic structure from a Mott insulator to a metallic state through selection of substrate lattice mismatches and reducing film thicknesses, and found the simultaneous increase in $|S|$ and $\sigma$ is realized by large enhancement of carrier mobility beyond the Mott insulator to metal transition, boosting the power factor by more than 2 orders of magnitude. Our experiments suggest that epitaxial strain will be an ideal tool.

![Figure 4](www.advancedsciencenews.com)
to finely tune materials close to their Mott transition, and thus to harvest large power factors from TMOs that are inconspicuous in their bulk.

4. Experimental Section

**Thin Film Growth:** LTO epitaxial films were grown on (001) pseudo-cubic perovskite substrates of YAlO$_3$, LaAlO$_3$, LSAT, DyScO$_3$, GdScO$_3$, and NdScO$_3$ (10 × 10 × 0.5 mm$^3$) by pulsed laser deposition. A KrF excimer laser ($λ = 248$ nm) was used to ablate a La$_2$Ti$_2$O$_7$ polycrystalline target disk, with a laser energy fluence and repetition rate of $1 \text{ J cm}^{-2}$ and 2 Hz, respectively. Films were deposited in vacuum ($\approx 1 \times 10^{-3}$ Pa) at a growth temperature of 780 °C. After deposition, films were cooled to RT in vacuum.

**Structural and Chemical Analysis:** The crystal structures were investigated by high-resolution XRD (anode radiation: monochromatic CuKα) at RT (Figures S1–S3, Supporting Information). Atomic force microscopy (AFM) revealed atomically flat surfaces with step-and-terrace structures (Figure S4, Supporting Information). TEM samples with 50 nm thick LTO films on LaAlO$_3$ substrate were prepared by mechanical polishing with cooling water and thinned by Cryo ion slicer with a holding temperature of $-150$ °C at $\approx 10^{-3}$ Pa. The cross-sectional microstructure of the LTO film was examined at RT by HAADF-STEM (JEM-ARM200F, 200 kV, JEOL), with electron incident direction LaAlO$_3$ [100]. Dominance of the Ti$^{3+}$ valence state was confirmed by EELS in conjunction with HAADF-STEM that also attested the sharpness of the LTO/LaAlO$_3$ interface (Figures S5–S7, Supporting Information). HAADF-STEM images were taken with the detection angle of 68–280 mrad, and the EELS were acquired by Enfinium spectrometer (Gatan Inc.) with the energy resolution of about 1 eV. Homogeneity of the La, Ti, and O chemical compositions was verified by FE-AES along the depth direction (Figure S5e, Supporting Information). HAADF-STEM images were taken with the detection angle of 68–280 mrad, and the EELS were acquired by Enfinium spectrometer (Gatan Inc.) with the energy resolution of about 1 eV. Homogeneity of the La, Ti, and O chemical compositions was verified by FE-AES along the depth direction (Figure S5e, Supporting Information).

**Electrical Transport Measurement:** $σ$ was measured by a d.c. four-probe method with the van der Pauw electrode configuration. $σ$ was measured by applying temperature gradient ($ΔT$) of $≈ 4$ K while the actual temperatures of both sides of the film surface were monitored by thermocouples. The thermo-electromotive force ($ΔV$) and $ΔT$ were simultaneously measured, and $σ$ was obtained from the slope of the $ΔV$–$ΔT$ plots.

**First-Principles Calculation:** The stable structure of LTO under epitaxial strain and their electronic structures were examined by first-principles calculations. All structural relaxations are performed within the generalized gradient approximation (GGA, in the Perdew–Burke–Ernzerhof (PBE) realization) of DFT using the QUANTUM ESPRESSO code [37] which implements the plane-wave pseudo-potential method. We employed pseudo-potentials from the SSSP library [38] with an energy cutoff of 50 Ry. Structural relaxations of LTO under different epitaxial constraints were simulated using a conventional cell containing 20 atoms with a Γ-centered 9 × 9 × 6 k-point mesh. For each strain, we fixed the in-plane lattice parameter and relaxed the out-of-plane lattice parameter $c$ as well as all internal positions. The results were double checked with the GGA-PBEsol functional (Figure S8, Supporting Information). Strain dependencies of nearest-neighbor hopping parameters and on-site energies of the Ti 3d $t_{2g}$ orbitals were evaluated from maximally localized Wannier functions from Wannier90 [39] using Kohn-Sham states within $-1 \text{ eV} - +6 \text{ eV}$ around the $E_F$, and frozen windows within $-1$ to $-0.35 \text{ eV}$ and $1$ to $+0.1 \text{ eV}$ for I4/mcm and I4/mmm structures, respectively.

Figure 5. a) Thermopower ($S$) as a function of electrical conductivity ($σ$), b) weighted mobility ($\mu_w$) versus $σ$, and c) $S$ versus carrier concentration ($n_w$) calculated by $n_w = σ / (\epsilon \mu_w)$ at room temperature for LTO films with thickness of 50 nm on YAIo$_3$ (open pink symbols), LaAlO$_3$ (open red symbols), LSAT (open purple symbols), DyScO$_3$ (open bright yellow symbols), GdScO$_3$ (open green symbols), NdScO$_3$ (open blue symbols), and those with thicknesses of 4–100 nm on LaAlO$_3$ substrate (closed red circles). Red (blue) delimits the region of n-type (p-type) charge polarity.
Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
Research data are not shared.

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