

Supporting Information

Improved Thermoelectric Properties of SrTiO₃ via (La, Dy and N) Co-Doping: DFT Approach

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Table S1. Amount of doping of La, Dy and N in SrTiO₃.

Systems	Number of atoms						Chemical formula
	Sr	Ti	O	La	Dy	N	
Pristine SrTiO ₃	8	8	24	-	-	-	SrTiO ₃
12.5% of La-doped SrTiO ₃	7	8	24	1	-	-	Sr _{0.875} La _{0.125} TiO ₃
12.5% of Dy-doped SrTiO ₃	7	8	24	-	1	-	Sr _{0.875} Dy _{0.125} TiO ₃
4.2% of N-doped SrTiO ₃	8	8	23	-	-	1	SrTiO _{2.958} N _{0.042}
(La, Dy)-co doped SrTiO ₃	6	8	24	1	1	-	Sr _{0.750} La _{0.125} Dy _{0.125} TiO ₃
(La, N)-co doped SrTiO ₃	7	8	23	1	-	1	Sr _{0.875} La _{0.125} TiO _{2.958} N _{0.042}

Table S2. Total energy (E_{tot}), total energy per atom (E_{atom}), and formation energy (E_{form}) of the host sites replaced by La, Dy and N atoms. The number in the parentheses gives the total number of atoms in the bulk structure. The bold numbers for E_{form} representing the lowest values, indicating the most stable structures in experiments.

Bulk structures	E_{tot} (eV)	E_{atom} (eV)
Sr (2 Atoms)	-3.08	-1.54
Ti (3Atoms)	-23.59	-7.86
O (8 Atoms)	-39.52	-4.94
La (4 Atoms)	-20.65	-5.16

Dy (3 atoms)	-13.63	-4.54
N (2 atoms)	-16.54	-8.27
Undoped STO	-320.80	

Structure	E_{tot} (eV)	E_{form} (eV)
La-doped STO		
1. Sr replaced by La	-325.17	-0.75
2. Ti replaced by La	-312.41	5.69
3. O replaced by La	-307.65	13.38
Dy-doped STO		
1. Sr replaced by Dy	-323.87	-0.06
2. Ti replaced by Dy	-314.44	3.04
3. O replaced by Dy	-307.76	12.64
N-doped STO		
1. Sr replaced by N	-312.02	15.52
2. Ti replaced by N	-305.05	16.16
3. O replaced by N	-318.84	5.29

The formation energy is calculated using the equation

$$E_f = E_{\text{doped STO}} - E_{\text{STO}} - nE_{\text{doped atom}} + nE_{\text{host}},$$

where $E_{\text{doped STO}}$, E_{STO} , $E_{\text{doped atom}}$, and E_{host} donate the total energy of the doped STO, the undoped STO, the atom doping into STO calculated from bulk structures, and the host atom doping calculated from bulk structures, respectively. Moreover, n is the number of atoms added or removed from the pristine STO to design the (La, Dy and N)-mono-doped STO.^{1,2}

Table S3. Lattice parameters of the most stable structures for undoped and doped SrTiO₃.

Systems	a (Å)	b (Å)	c (Å)	alpha (°)	beta (°)	gamma (°)
Pristine SrTiO ₃	7.880	7.880	7.880	90.00	90.00	90.00
12.5% of La-doped SrTiO ₃	7.883	7.883	7.883	90.00	90.00	90.00
12.5% of Dy-doped SrTiO ₃	7.863	7.863	7.863	90.00	90.00	90.00
4.2% of N-doped SrTiO ₃	7.889	7.889	7.900	90.00	90.00	90.00
(La, Dy)-co doped SrTiO ₃	7.851	7.873	7.873	90.00	90.00	90.00
(La, N)-co doped SrTiO ₃	7.876	7.906	7.906	89.76	90.00	90.00

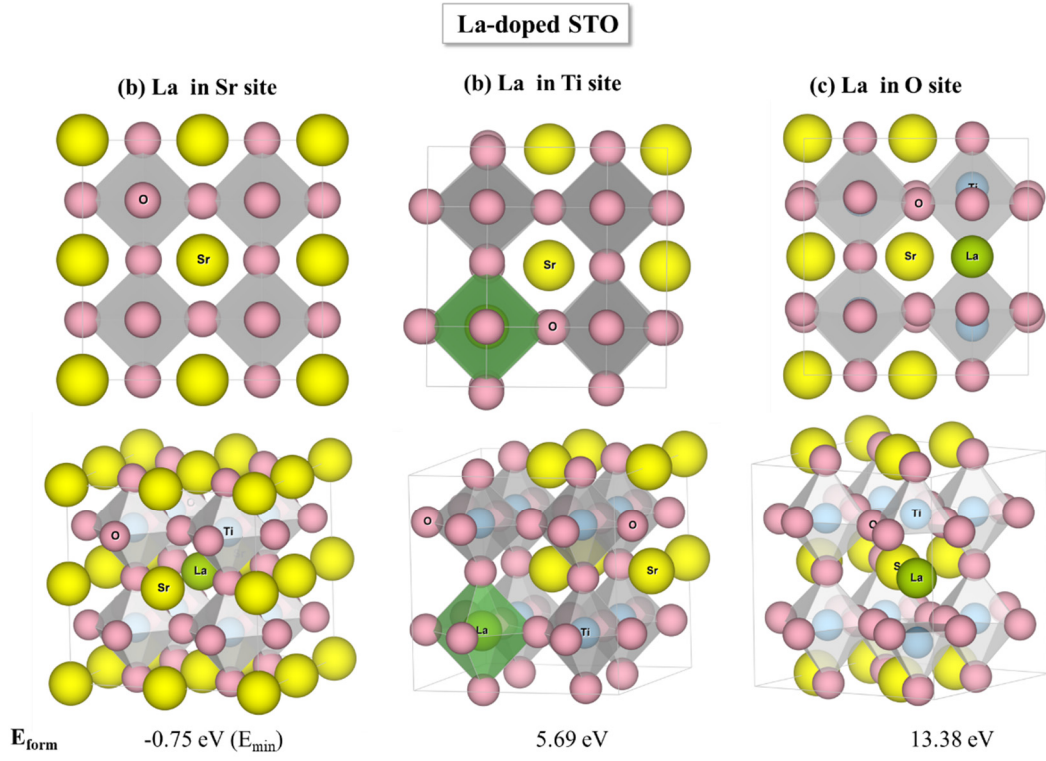


Figure S1. The optimized structures of La-doped SrTiO_3 after replacing La atoms in Sr, Ti, and O sites with formation energy (E_{form}) as the total energy as listed in Table S2. The pink spheres are the O atoms, yellow are Sr, light blue are Ti, and green are La. E_{min} indicates the structure providing the lowest formation energy.

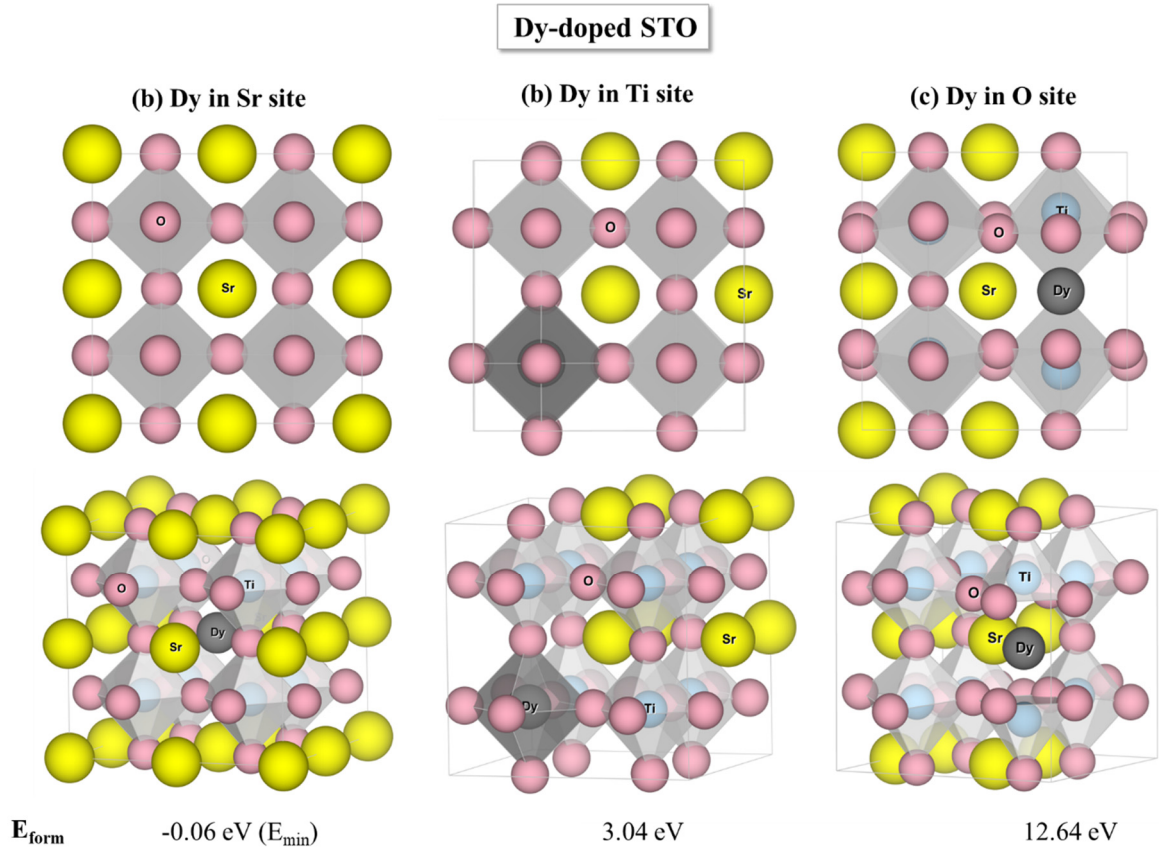


Figure S2. The optimized structures of Dy-doped SrTiO_3 after replacing Dy atoms in Sr, Ti, and O sites with formation energy (E_{form}) as the total energy as listed in Table S2. The pink spheres are the O atoms, yellow are Sr, light blue are Ti, and grey are Dy. E_{min} indicates the structure providing the lowest formation energy.

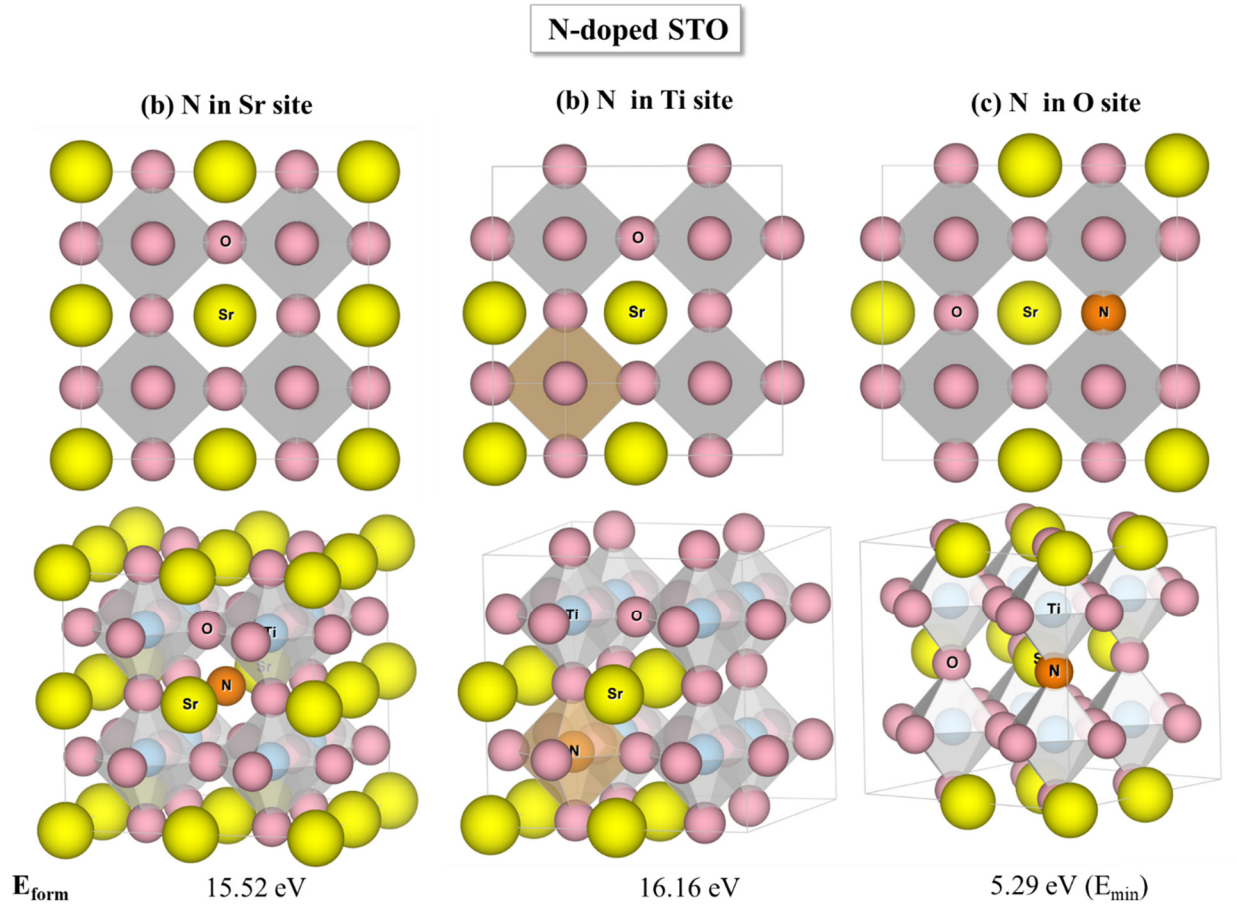


Figure S3. The optimized structures of N-doped SrTiO_3 after replacing N atoms in Sr, Ti, and O sites with formation energy (E_{form}) as the total energy as listed in Table S2. The pink spheres are the O atoms, yellow are Sr, light blue are Ti, and orange are N. E_{min} indicates the structure providing the lowest formation energy.

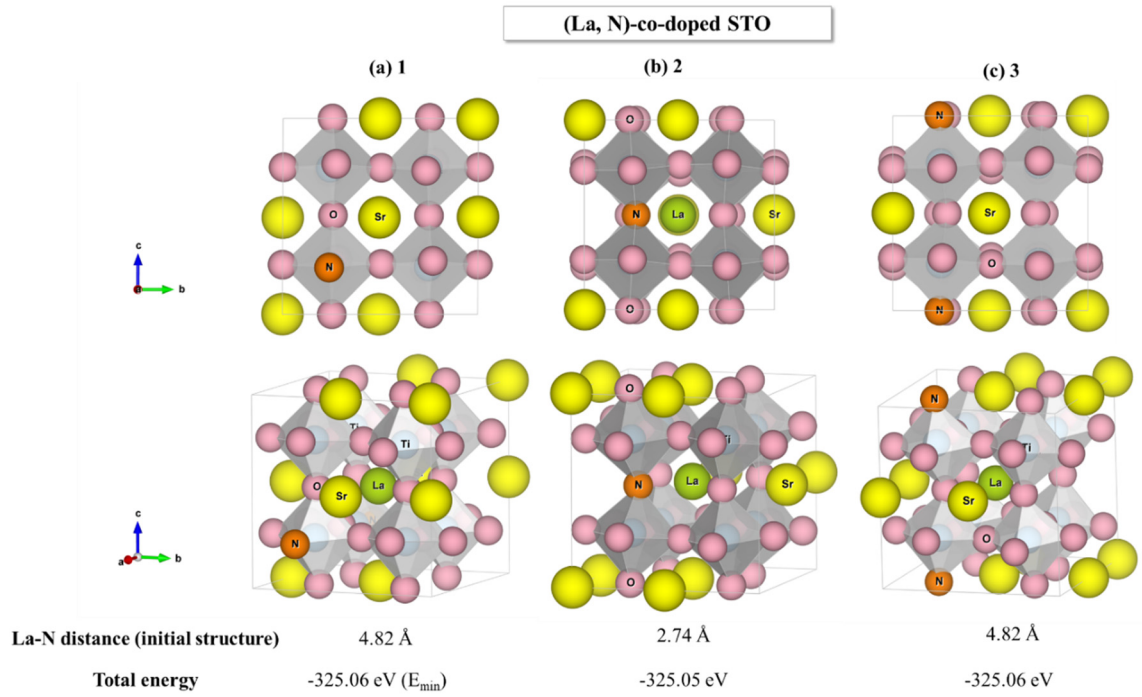


Figure S4. Three different La-N distances, with the total energy of the supercell configuration, for 3 different sites of La and N doping, in which both La and N atoms replace Sr and O sites, respectively. $E_{\min}$ indicates the structure providing the lowest total energy, which is the most stable structure.

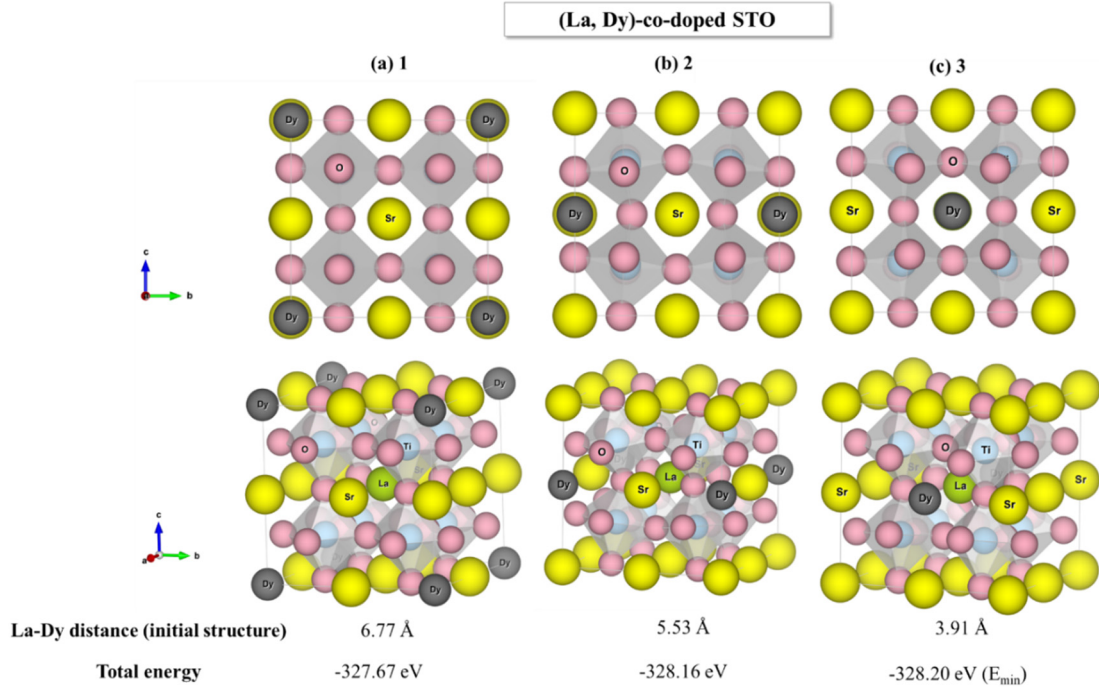


Figure S5. Three different La-Dy distances, with the total energy of the supercell configuration, for 3 different sites of La and Dy doping, in which both La and Dy atoms replace Sr sites. $E_{\min}$ indicates the structure providing the lowest total energy, which is the most stable structure.

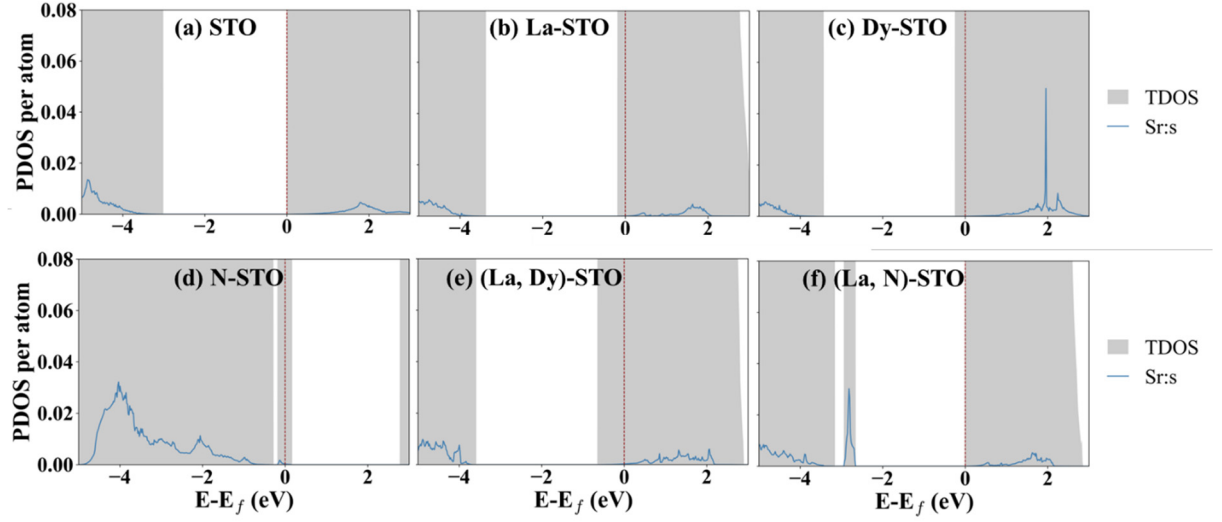


Figure S6. DOS of s orbitals of Sr for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

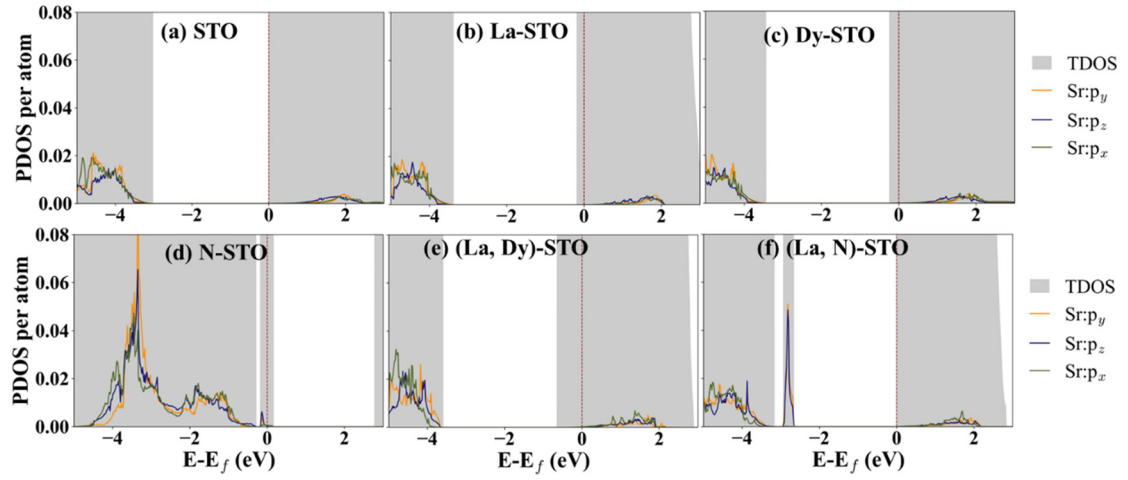


Figure S7. DOS of p orbitals of Sr for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

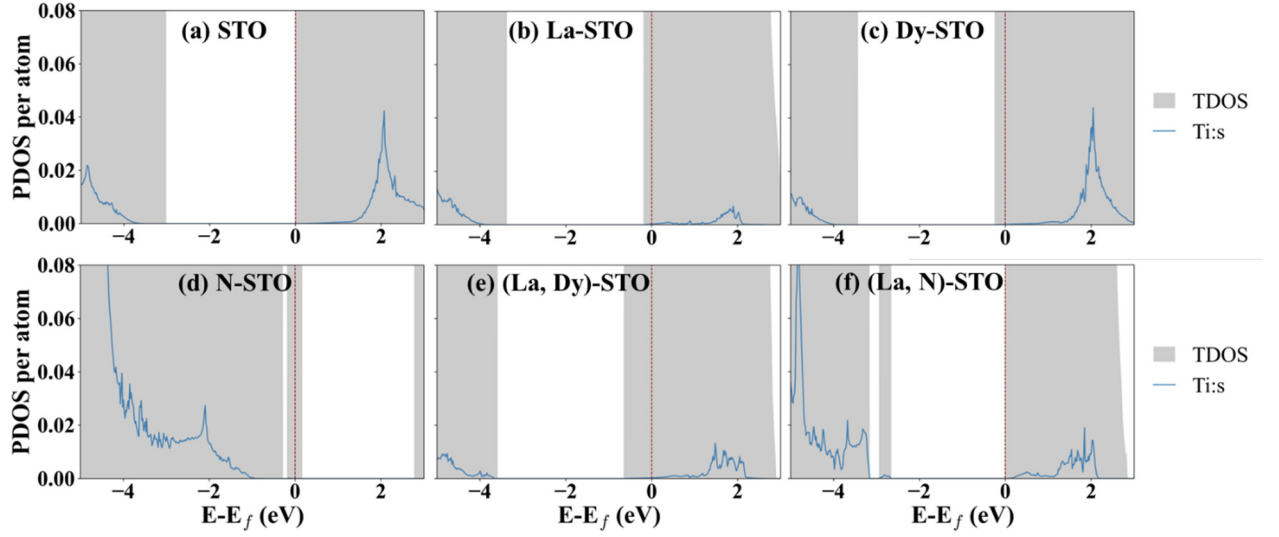


Figure S8. DOS of s orbitals of Ti for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

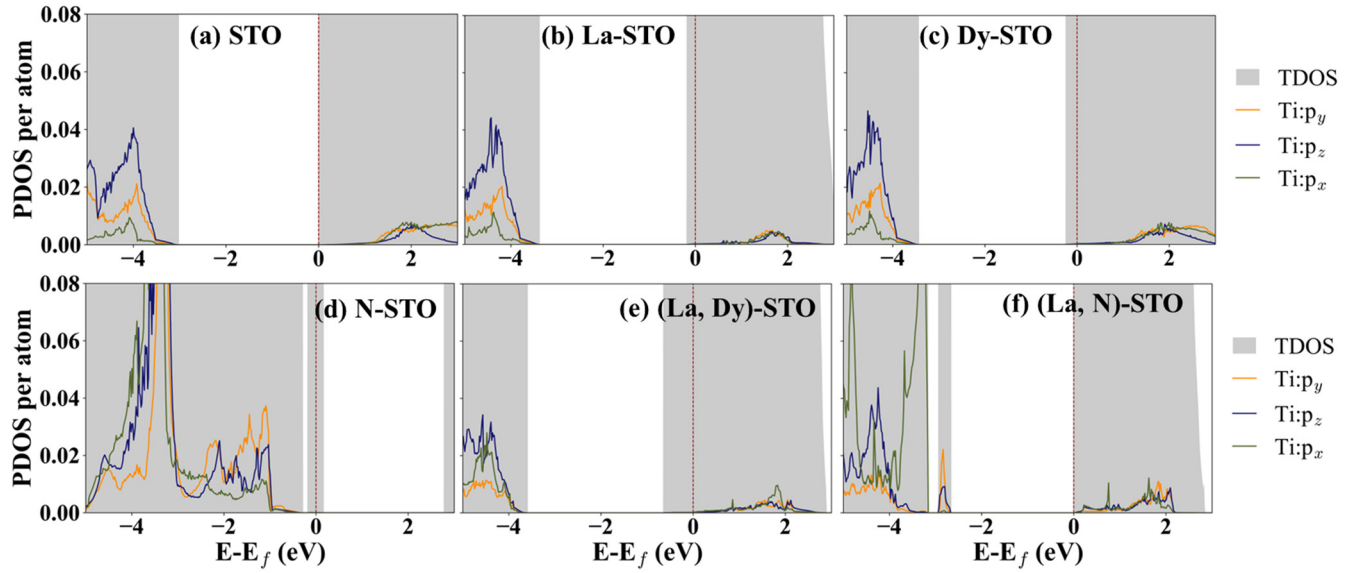


Figure S9. DOS of p orbitals of Ti for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

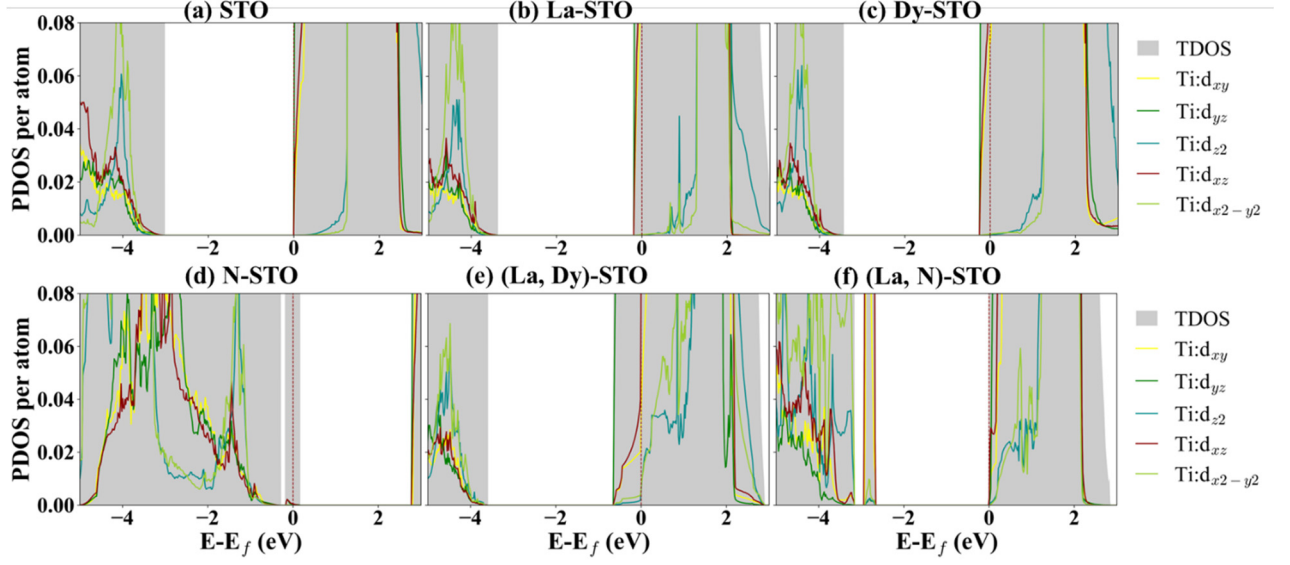


Figure S10. DOS of d orbitals of Ti for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

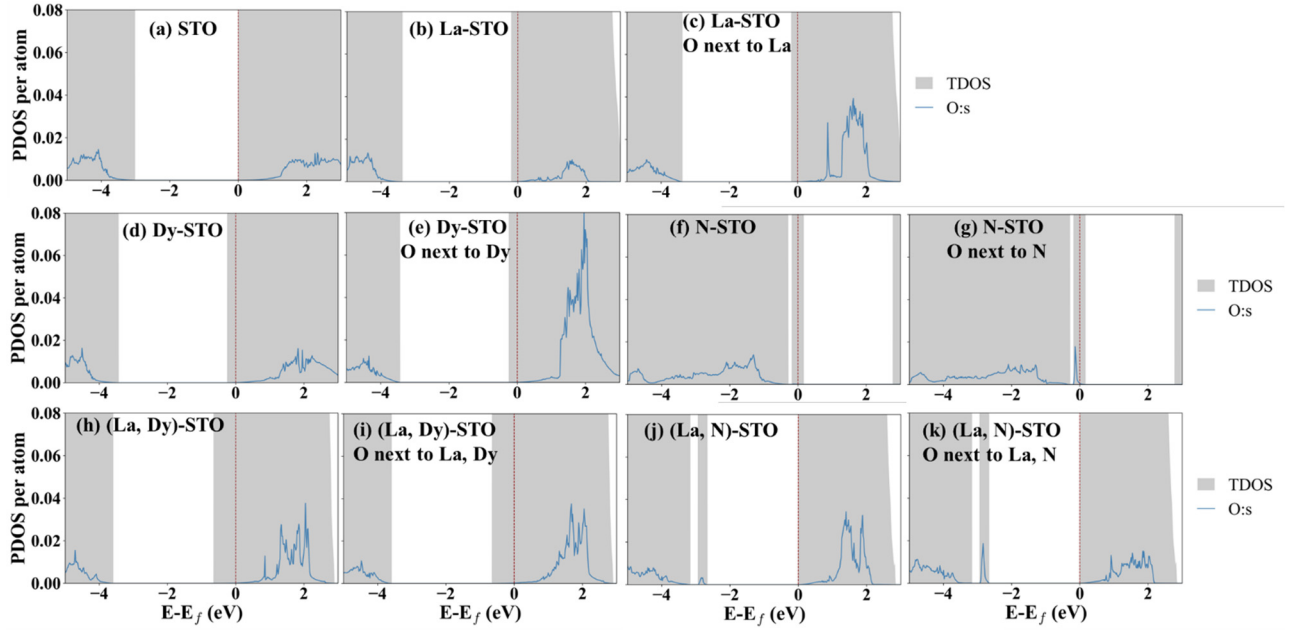


Figure S11. DOS of s orbitals of O for (a) undoped, (b, c) La-doped, (d, e) Dy-doped, (f, g) N-doped, (h, i) (La, Dy)-doped, and (j, k) (La, N)-doped SrTiO₃. Two O atoms are observed at positions which are (a, b, d, f, h, and j) remote from and (c, e, g, i, and k) neighboring the doped atoms.

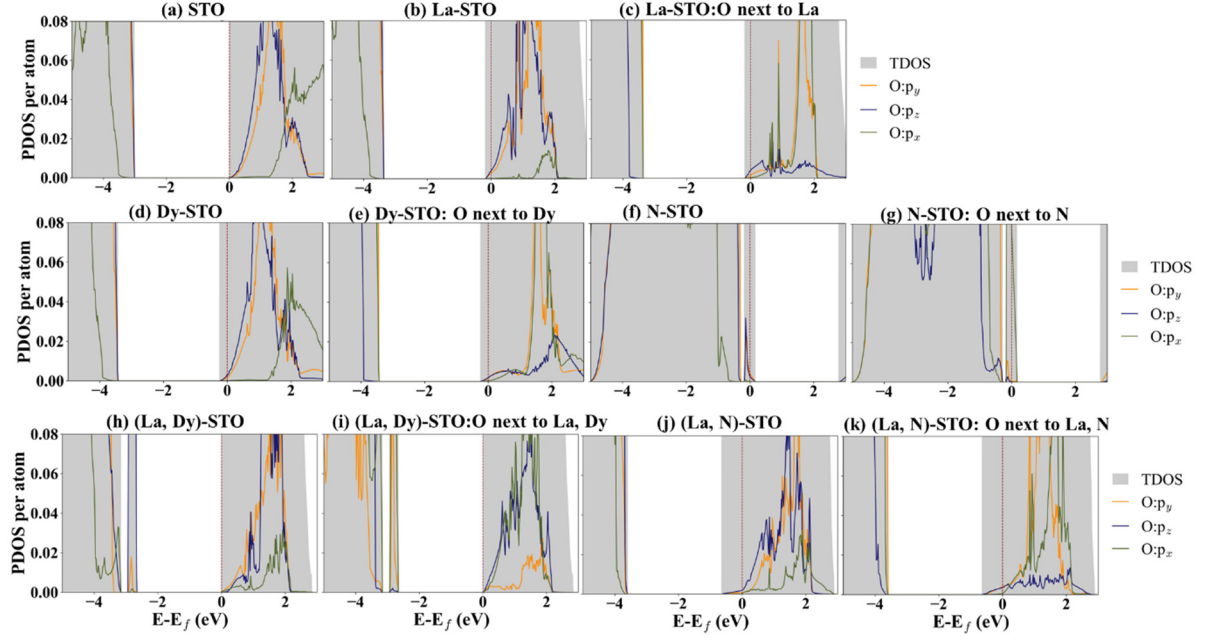


Figure S12. DOS of p orbitals of O for (a) undoped, (b, c) La-doped, (d, e) Dy-doped, (f, g) N-doped, (h, i) (La, Dy)-doped, and (j, k) (La, N)-doped SrTiO_3 . Two O atoms are observed at positions which are (a, b, d, f, h, and j) remote from and (c, e, g, i, and k) neighboring the doped atoms.

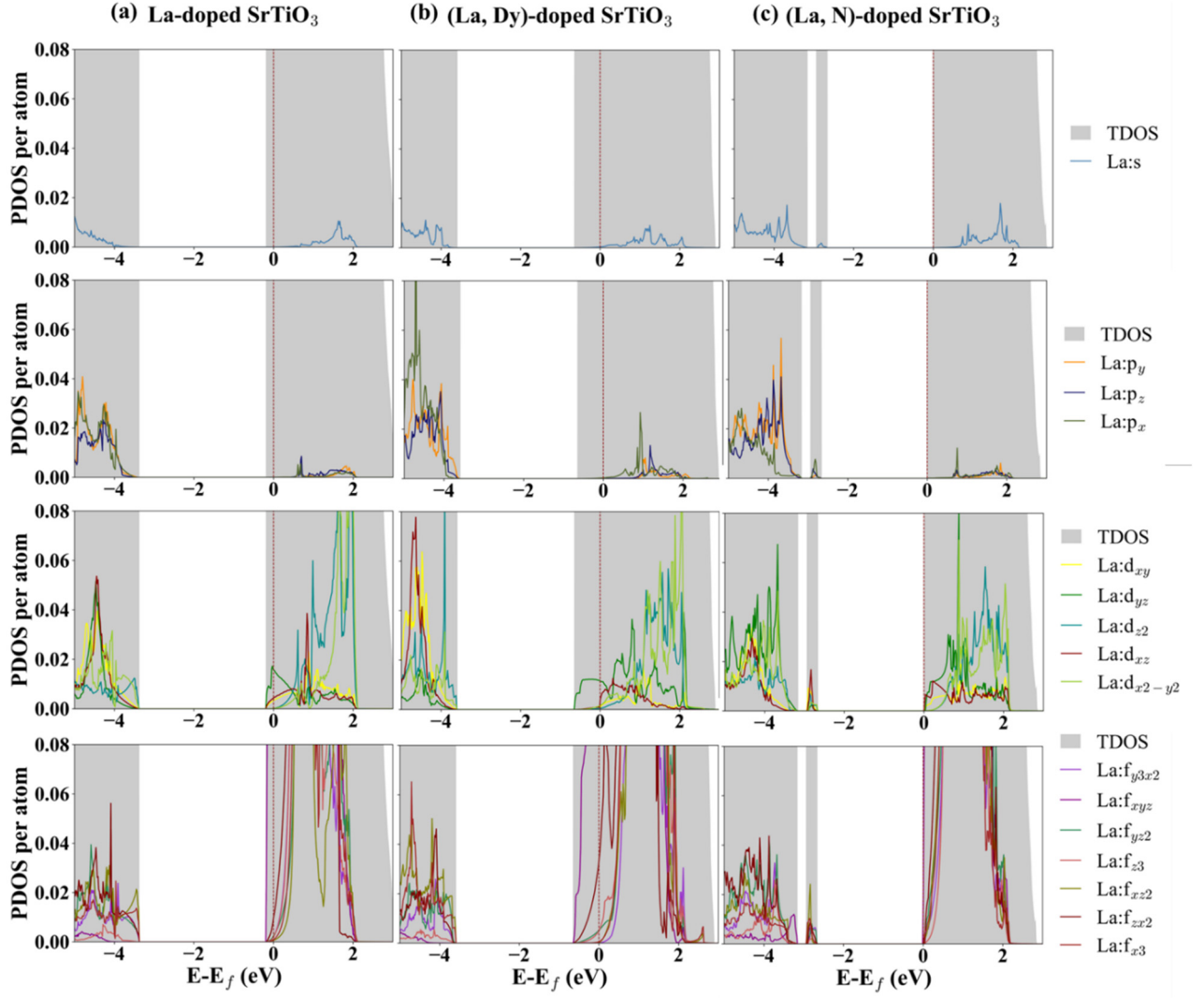


Figure S13. DOS of s , p , d and f orbitals of La for (a) La-doped, (b) (La, Dy)-doped, and (c) (La, N)-doped SrTiO₃.

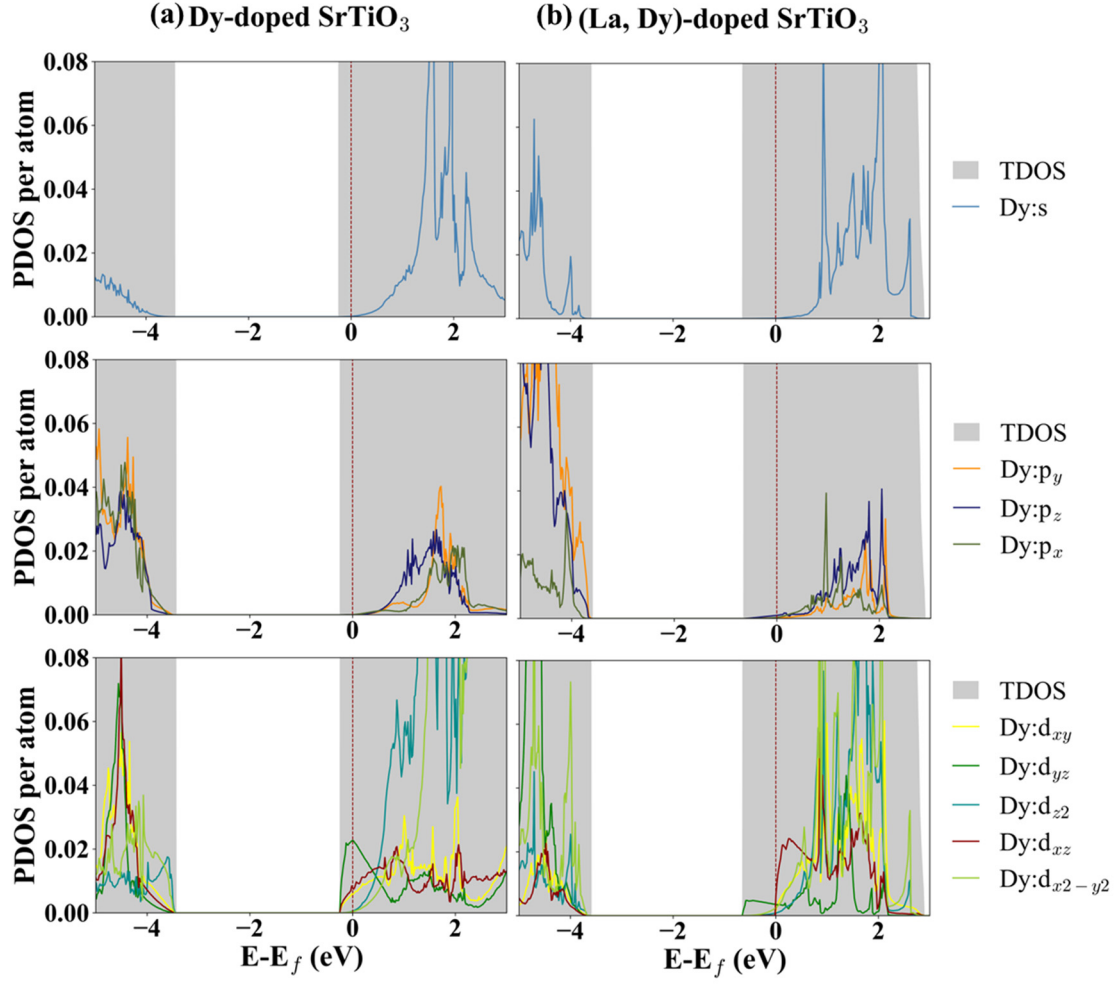


Figure S14. DOS of s , p , and d orbitals of Dy for (a) Dy-doped and (b) (La, Dy)-doped SrTiO_3 .

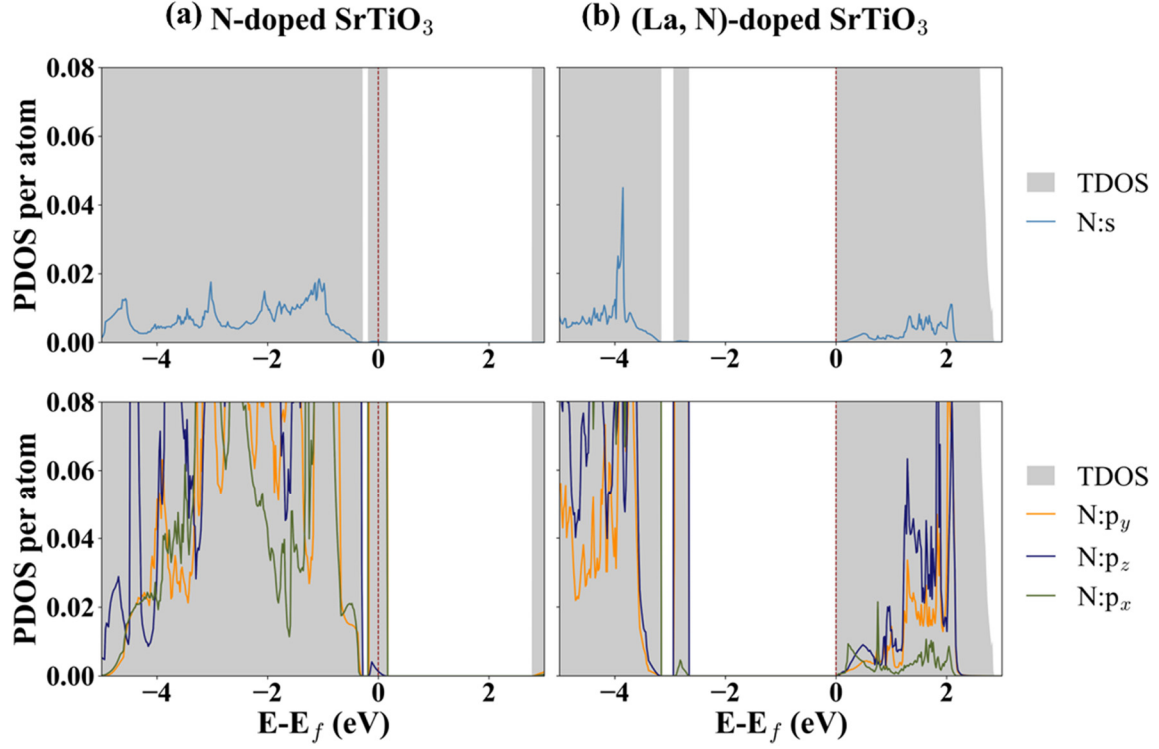


Figure S15. DOS of s and p orbitals of N for (a) N-doped and (c) (La, N)-doped SrTiO_3 .

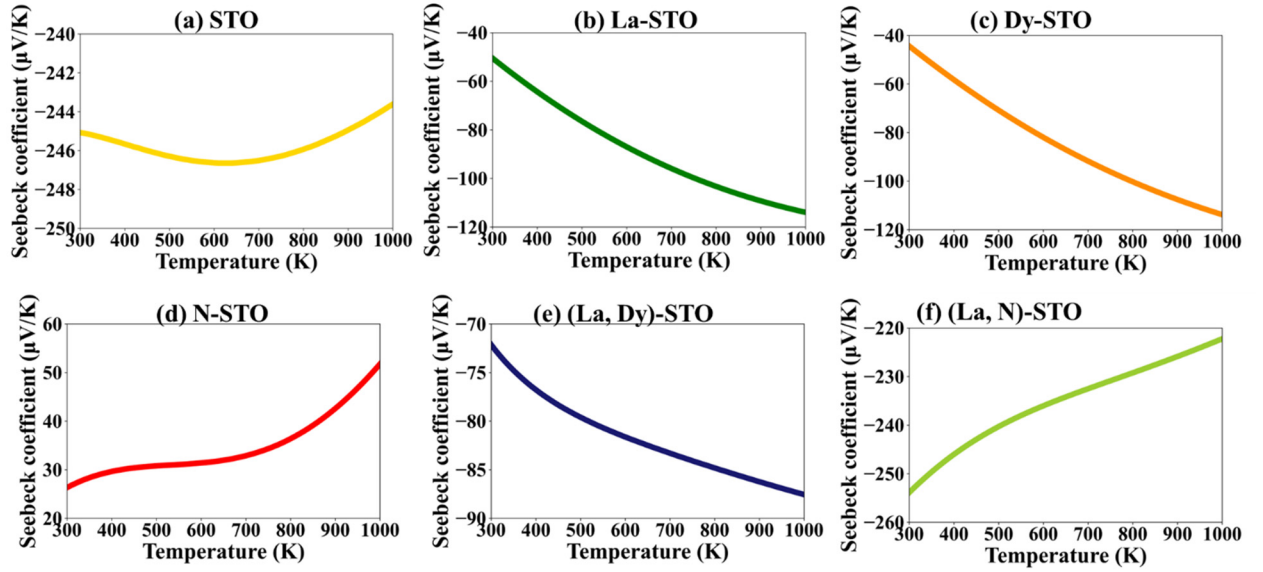


Figure S16. Seebeck coefficient versus temperature variation for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO_3 .

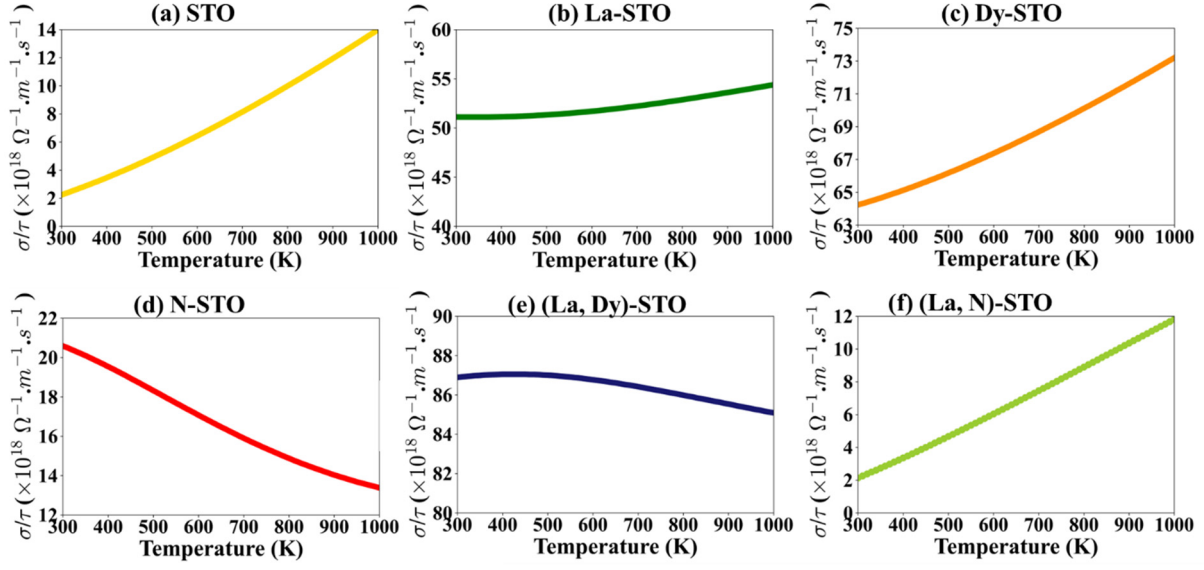


Figure S17. Ratio of electrical conductivity to relaxation time (σ/τ) with temperature variation for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

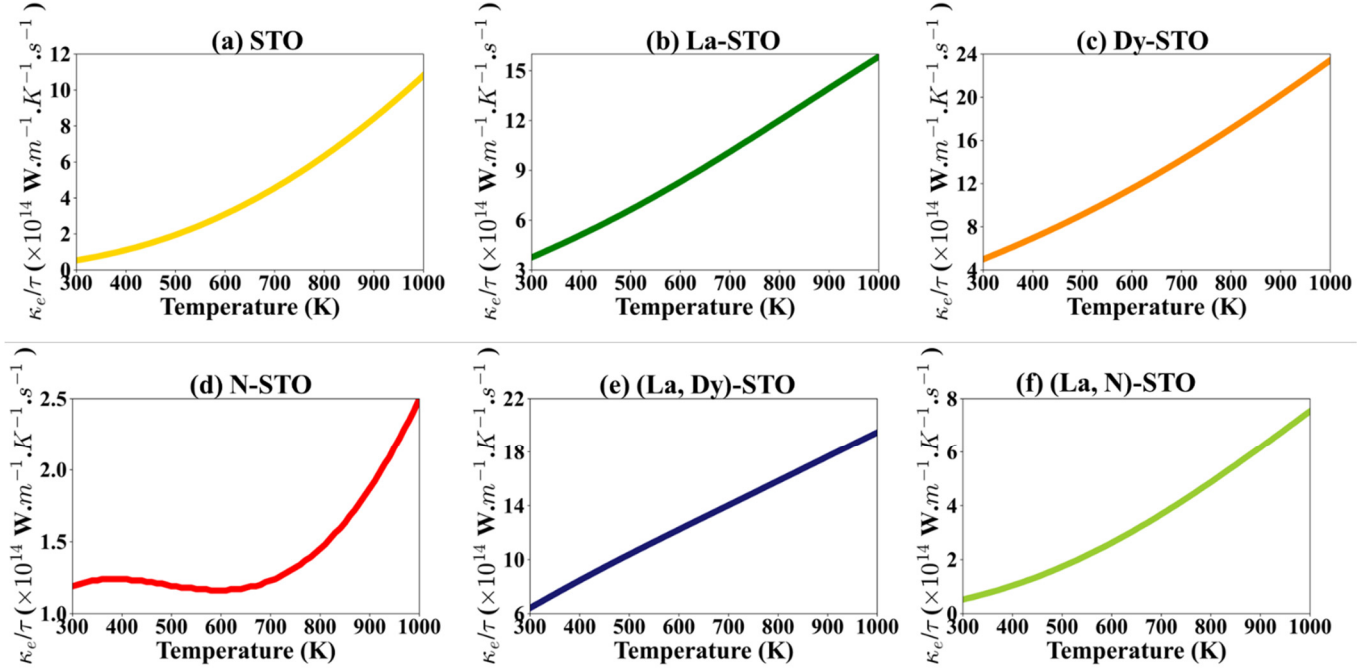


Figure S18. Ratio of electronic thermal conductivity to relaxation time (κ_e/τ) with temperature variation for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.

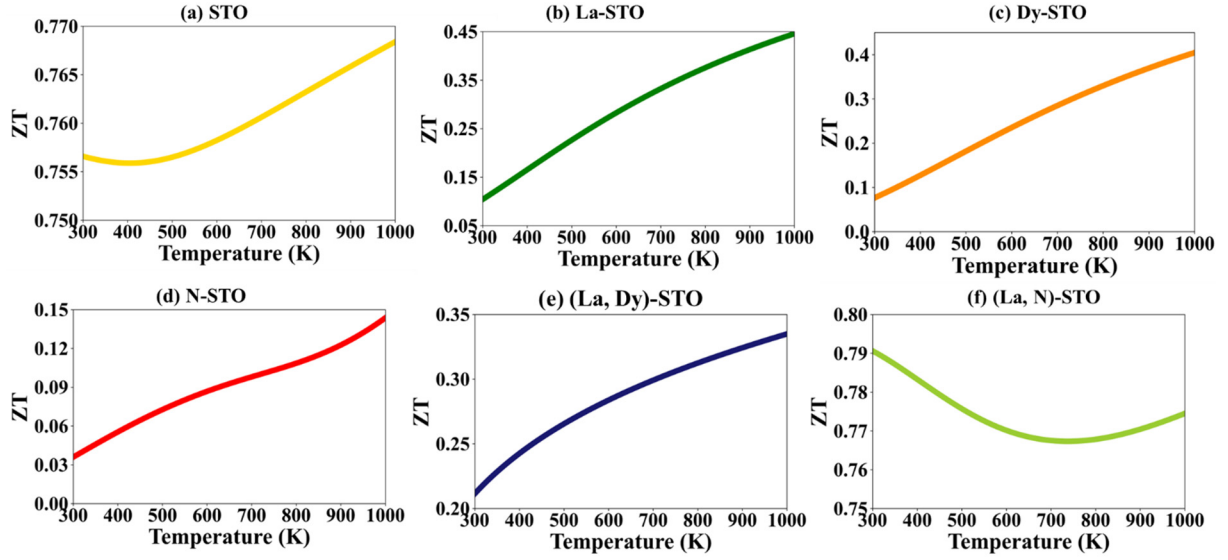


Figure S19. Figures of merit (ZT) versus temperature variation for (a) undoped, (b) La-doped, (c) Dy-doped, (d) N-doped, (e) (La, Dy)-doped, and (f) (La, N)-doped SrTiO₃.