Supplementary Materials.

1 Supplementary Figures and Tables

1.1 Supplementary Figures

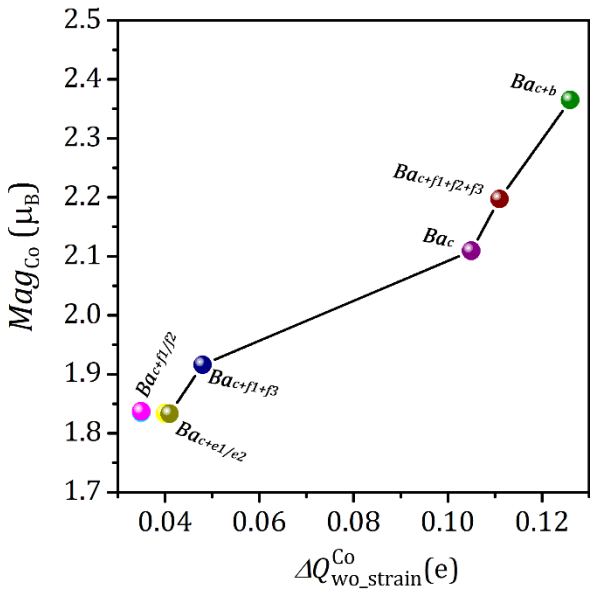

Figure S1. The magnetic moment localized at Co atoms Mag_{Co} versus charge variation in Co atom originating from the different electronic configuration between Ba and La $\Delta Q^{Co}_{wo\_strain}$.

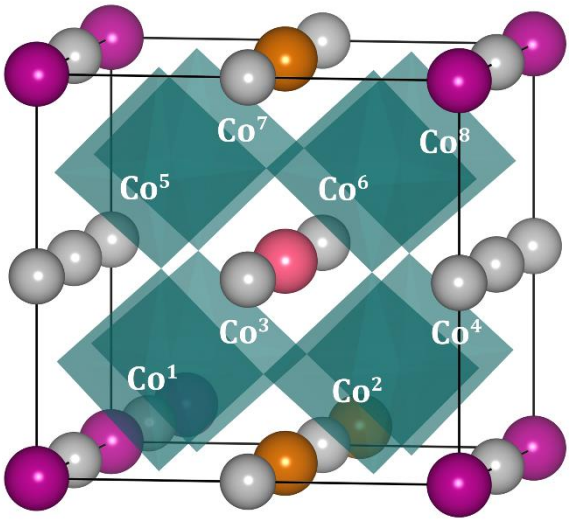

Figure S2. Optimized structure of Ba_{c+b+f1}.

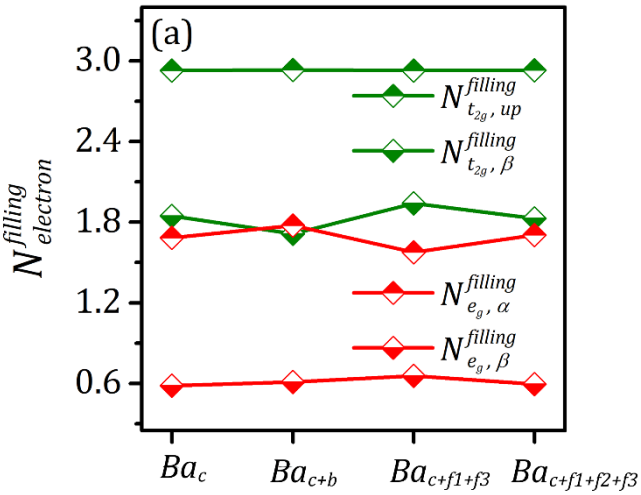

Figure S3. The t_{2g}, e_g-band filling for majority α-spin and minority β-spin, $N_{t_{2g},\alpha}^{filling}$, $N_{e_g,\alpha}^{filling}$, $N_{t_{2g},\beta}^{filling}$, $N_{e_g,\beta}^{filling}$, for Ba_c, Ba_{c+b}, $Ba_{c+f1+f3}$, and $Ba_{c+f1+f2+f3}$ modified $LaCoO_3$.

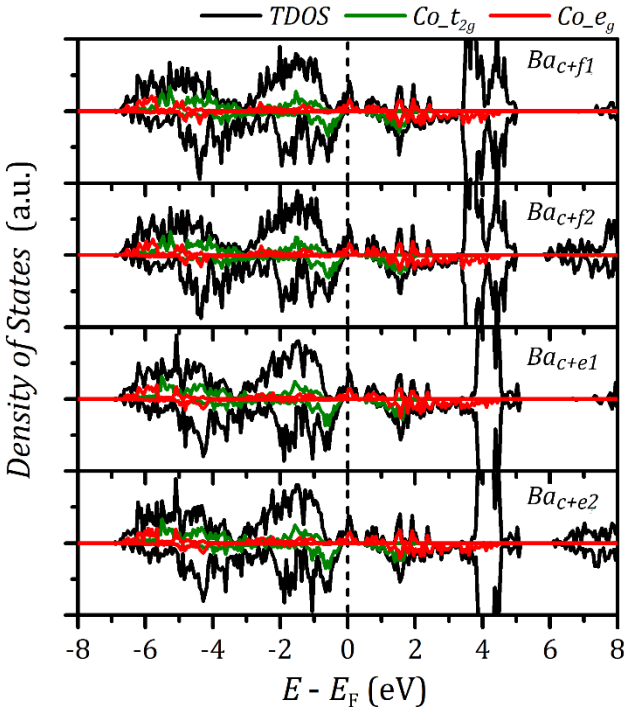

Figure S4. Projected density of state of Co atom and total density of states for Ba_{c+f1}, Ba_{c+f2}, Ba_{c+e1}, and Ba_{c+e2} defective $LaCoO_3$.

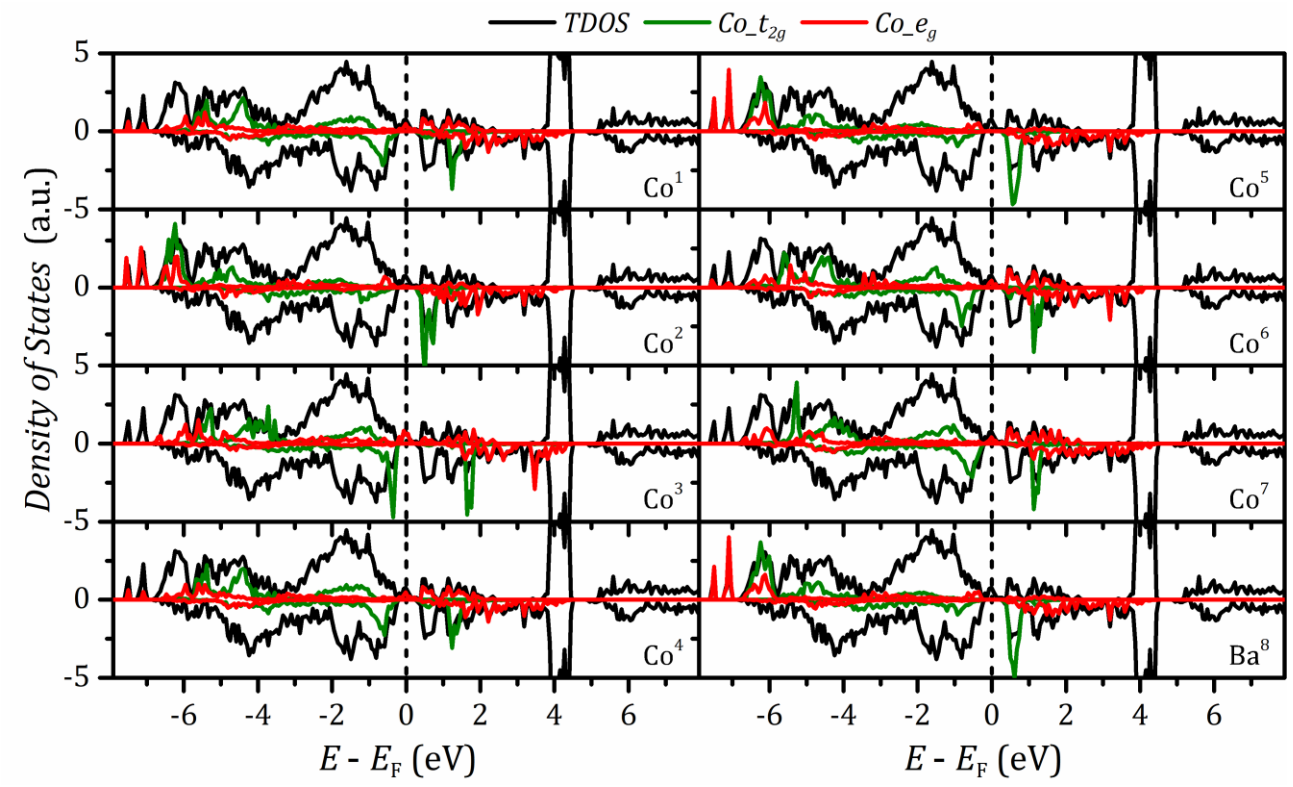

Figure S5. Projected density of states of Co^{i} (i=1, 2, 3, 4, 5, 6, 7, and 8) and total density of states for Ba_{c+b+f1} defective $LaCoO_3$.

1.2 Supplementary Tables

Table S1. The Magnetic moment localized at Co atom, Mag_{Co} in μ_B, calculated with U_{eff} of 2.8, 3.0 3.5, 3.8, and 4.0 eV, for pristine $LaCoO_3$ under γ = 0.0%, 2.0%, and 8.0%.

	U_{eff}					
	2.8	***3.0***	***3.3***	***3.5***	***3.8***	***4.0***
γ = 0.0%	0.000	0.000	0.000	0.000	0.000	0.000
γ = 2.0%	1.407	1.392	1.405	1.390	1.405	1.415
γ = 8.0%	2.569	2.581	2.598	2.610	2.626	2.637

Table S2. The Magnetic moment localized at Co atom, Mag_{Co} in μ_B, and t_{2g}, e_g-band center for majority α-spin and minority β-spin, $\varepsilon_{t_{2g},\alpha}$, $\varepsilon_{e_g,\alpha}$, $\varepsilon_{t_{2g},\beta}$, $\varepsilon_{e_g,\beta}$, under various strain γ.

strain	Mag_{Co}	$\varepsilon_{t_{2g},\alpha}$	$\varepsilon_{t_{2g},\beta}$	$\varepsilon_{e_g,\alpha}$	$\varepsilon_{e_g,\beta}$
-4	0	-2.53659	-2.53659	-1.30237	-1.30257
-3	0	-2.45066	-2.45066	-1.09759	-1.09761
-2	0	-2.37887	-2.37887	-0.93281	-0.93277
-1	0	-2.20589	-2.20587	-0.69031	-0.69036
-0.9	0	-2.1935	-2.1935	-0.67151	-0.67158
-0.8	0	-2.16776	-2.16776	-0.62312	-0.62314
-0.7	0	-2.15602	-2.15602	-0.59872	-0.59869
-0.6	0	-2.1386	-2.13863	-0.5764	-0.57643
-0.5	0	-2.23248	-2.23244	-0.67199	-0.6721
-0.4	0	-2.21375	-2.21375	-0.63182	-0.63182
-0.3	0	-2.20166	-2.20166	-0.60767	-0.60765
-0.2	0	-2.18023	-2.18024	-0.59374	-0.59378
-0.1	0	-2.16504	-2.16503	-0.5886	-0.58859
0	0	-2.15824	-2.15824	-0.52247	-0.52248
0.1	0	-2.16634	-2.16633	-0.57113	-0.57113
0.2	0	-2.21429	-2.21429	-0.65343	-0.65341
0.3	0	-2.14687	-2.14687	-0.53945	-0.53945
0.4	0	-2.17987	-2.17987	-0.54111	-0.54111
0.5	0	-2.07225	-2.07225	-0.413	-0.41292
1	1.356	-2.68393	-1.17156	-2.21749	0.68943
1.5	1.37	-2.64496	-1.12206	-2.20369	0.75062
2	1.407	-2.64204	-1.07646	-2.22911	0.80175
2.5	1.421	-2.61277	-1.0348	-2.2171	0.86226
3	1.434	-2.5847	-1.00108	-2.18195	0.9323
3.5	1.448	-2.54867	-0.95489	-2.13976	1.01443
4	2.022	-3.19716	-0.80722	-3.1319	0.9711
5	2.16	-3.28791	-0.72425	-3.26372	1.03665
6	2.182	-3.15786	-0.62917	-3.29338	1.10159
7	2.271	-3.16211	-0.53382	-3.39751	1.15606
8	2.569	-3.51619	-0.45014	-3.90728	1.05309

9	2.58	-3.42934	-0.39218	-3.87453	1.12448
10	2.59	-3.36578	-0.35855	-3.88077	1.17916
11	2.6	-3.28912	-0.32854	-3.84874	1.24165
12	2.7	-3.42657	-0.23126	-4.05229	1.1893
13	2.776	-3.47579	-0.2123	-4.16697	1.14847
14	2.785	-3.39066	-0.19041	-4.14893	1.17933
15	2.79	-3.36436	-0.14288	-4.12741	1.21834
16	2.791	-3.26765	-0.11722	-4.12571	1.27301
17	2.795	-3.28018	-0.11137	-4.06536	1.3129
18	2.798	-3.20803	-0.05813	-4.10426	1.34925
19	2.8	-3.0859	0.01686	-4.1458	1.38082
20	2.801	-3.08143	0.01607	-4.09629	1.43372
25	2.84	-2.95108	0.19142	-4.15463	1.57409
30	2.791	-2.61248	0.277	-3.95783	1.8933

Table S3. The t_{2g}, e_g-band filling for majority α-spin and minority β-spin, $N_{t_{2g},\alpha}^{filling}$, $N_{e_g,\alpha}^{filling}$, $N_{t_{2g},\beta}^{filling}$, $N_{e_g,\beta}^{filling}$, under various strain γ.

Strain	$N_{t_{2g},\alpha}^{filling}$	$N_{t_{2g},\beta}^{filling}$	$N_{e_g,\alpha}^{filling}$	$N_{e_g,\beta}^{filling}$
-4	2.93627	2.93626	0.79969	0.79969
-3	2.93062	2.93064	0.77965	0.77965
-2	2.92714	2.92715	0.76246	0.76246
-1	2.93097	2.91978	0.74595	0.74595
-0.9	2.92198	2.92199	0.74486	0.74486
-0.8	2.92121	2.92121	0.74336	0.74336
-0.7	2.92195	2.92196	0.74114	0.74114
-0.6	2.91736	2.91733	0.7406	0.74062
-0.5	2.91916	2.91922	0.73911	0.73913
-0.4	2.92107	2.92108	0.73753	0.73752
-0.3	2.9194	2.9194	0.73547	0.73547
-0.2	2.91877	2.91876	0.73435	0.73435
-0.1	2.91851	2.91851	0.73315	0.73314
0	2.91866	2.91866	0.73191	0.73191
0.1	2.91825	2.91823	0.73054	0.73053
0.2	2.90492	2.90492	0.73981	0.7398
0.3	2.91652	2.91653	0.72754	0.72753
0.4	2.91666	2.91666	0.72637	0.72637
0.5	2.91468	2.91466	0.72509	0.72508
1	2.91636	2.11778	1.39098	0.54924
1.5	2.91448	2.18885	1.39416	0.53729
2	2.91315	2.12807	1.40253	0.52741
2.5	2.91114	2.04413	1.40369	0.51559
3	2.91096	2.08111	1.40902	0.50448
3.5	2.90792	2.0224	1.41046	0.49385
4	2.91393	1.80787	1.65221	0.48093
5	2.90924	1.77744	1.69819	0.46698
6	2.90996	1.69066	1.70417	0.4495
7	2.90909	1.62366	1.72193	0.43638

8	2.91007	1.51543	1.83328	0.44673
9	2.90872	1.56846	1.84683	0.43238
10	2.90663	1.52237	1.85226	0.41765
11	2.9056	1.61446	1.85117	0.40445
12	2.90529	1.57495	1.87281	0.40972
13	2.90553	1.54847	1.9027	0.41507
14	2.9027	1.57606	1.91033	0.40499
15	2.90236	1.49852	1.9063	0.39392
16	2.90048	1.60184	1.91206	0.38358
17	2.90057	1.56654	1.91248	0.37338
18	2.90035	1.51958	1.91276	0.36314
19	2.90137	1.46276	1.9123	0.35282
20	2.89681	1.4427	1.91269	0.34312
25	2.89926	1.44518	1.94127	0.30777
30	2.88421	1.55896	1.95551	0.23908

Table S4. The magnetic moment localized at each Co atom (Co^i, i=1, 2, 3, 4, 5, 6, 7, and 8), Mag_{Co} in μ_B, and charge transfer of each Co atom, ΔQ^{Co}, $\Delta Q^{Co}_{ref,pristine}$, and $\Delta Q^{Co}_{wo\_strain}$, for Ba_{c+b+f1} defective $LaCoO_3$ ($\Delta Q^{Co}_{ref,pristine}$ is the charge transfer of Co atom relative to the pristine strain-free $LaCoO_3$. $\Delta Q^{Co}_{wo_strain}$is the charge transfer of Co atom in defective $LaCoO_3$ due to the difference of electronic configuration between Ba and La).

	Co^1	Co^2	Co^3	Co^4	Co^5	Co^6	Co^7	Co^8
Mag_{Co}	1.781	2.059	2.761	1.783	2.757	1.606	1.752	2.758
ΔQ^{Co}	1.428	1.494	1.390	1.428	1.495	1.433	1.412	1.494
$\Delta Q^{Co}_{ref,pristine}$	0.074	0.139	0.036	0.073	0.140	0.078	0.057	0.139
$\Delta Q^{Co}_{wo\_strain}$	0.037	0.130	0.032	0.040	0.140	0.037	0.020	0.132