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Ferromagnetic behavior induced by La-doping in $SrCo_2As_2$

Supporting Information

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Table S1. Summary of Rietveld refinement parameters for nominal $Sr_{1-x}La_xCo_2As_2$(x = 0, 0.025, 0.05, 0.075, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0).

x	0	0.025	0.05	0.075	0.1	0.2	0.3
Main phase (mole ratio)	100%	>99.0%	>99.0%	>99.0%	>99.0%	>99.0%	>99.0%
LaOCoAs (mole ratio)	0	<1.0%	<1.0%	<1.0%	<1.0%	<1.0%	<1.0%
Space group	*I*4/*mmm* (No. 139)						
a (Å)	3.9439(1)	3.9466(2)	3.9475(1)	3.9479(1)	3.9486(2)	3.9512(2)	3.9590(1)
c (Å)	11.8126(3)	11.7786(5)	11.7557(4)	11.7422(4)	11.7290(6)	11.6430(6)	11.5260(4)
V (Å^3)	183.74(1)	183.45(1)	183.19(1)	183.02(2)	182.87(2)	181.77(1)	180.66(1)
Z_{As}	0.3582 (1)	0.3573(1)	0.3581(1)	0.3575(1)	0.3572(1)	0.3571(1)	0.3577(1)
Co-Co (Å)	2.7888(1)	2.7906(1)	2.7913(1)	2.7916(1)	2.7921(1)	2.7939(1)	2.7995(1)
As-Co-As (°)	107.21(1) × 4	106.91(2)	107.04(2)	106.87(2)	106.77(2)	106.55(2)	106.40(2)
	114.10 (1) × 2	114.72(2)	114.45(2)	114.82(2)	115.03(2)	115.48(2)	115.80(2)
Co-As-Co (°)	72.79 (1)	73.09(2)	72.96(1)	73.14(1)	73.23(2)	73.45(2)	73.60(2)
Diffractometer	PANalyitical X'Pert Pro						
Radiation type	Co Kα						
Wavelength (Å)	1.79026						
Collection Range (° 2θ)	10 to 130						
Step size (° 2θ)	0.017						
Number of Observations (N)	7059	7059	7059	7059	7059	7059	7059
Number of structure parameters ($P1$)	4	4	4	4	4	4	4
Number of profile parameters ($P2$)	9	9	9	9	9	9	9
R_p	2.87%	3.58%	2.90%	3.19%	3.47%	4.12%	3.62%
R_{wp}	3.79%	4.92%	4.00%	4.53%	4.89%	5.86%	5.15%
R_{exp}	1.79%	1.48%	1.59%	1.57%	1.58%	1.59%	1.64%

χ^2	4.50	11.0	6.29	8.27	9.62	13.5	9.87

Note: $R_p=\sum|y_{io}-y_{ic}|/\sum|y_{io}|$, $R_{wp}=[\sum w_i(y_{io}-y_{ic})^2/\sum w_i y_{io}^2]^{1/2}$, $R_{exp}=[\ (N-P_1-P_2)/\sum w_i y_{io}^2]^{1/2}$, $\chi^2=\sum[w_i(y_{io}-y_{ic})^2/(N-P_1-P_2)\ ]^{1/2}$.

x	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Main phase (mole ratio)	99.0%	>99.0%	>99.0%	97.4%	>99.0%	98.4%	90.7%
LaOCoAs (mole ratio)	1.0%	<1.0%	<1.0%	2.6%	<1.0%	1.6%	9.3%
Space group	*I*4/*mmm* (No. 139)						
a (Å)	3.9711(2)	3.9768(1)	3.9988(1)	4.0096(2)	4.0210(2)	4.0378(2)	4.0449(2)
c (Å)	11.3803(1)	11.3002(7)	11.0502(4)	10.9318(8)	10.8019(8	10.6085(5)	10.4999(7
V (Å^3)	179.46(1)	178.71(1)	176.70(1)	175.75(2)	174.65(2)	172.96(1)	171.80(2)
Z_{As}	0.3578(1)	0.3588(1)	0.3590(1)	0.3615(1)	0.3608(2)	0.3604(1)	0.3616(1)
Co-Co (Å)	2.8080(1)	2.8120(1)	2.8276(1)	2.8352(2)	2.8433(1)	2.8551(1)	2.8602(1)
As-Co-As (°)	106.04(3) × 4	106.06(3)	105.44(2)	105.67(3)	105.17(4)	104.58(3)	104.55(3)
	116.58(3) × 2	116.53(3)	117.87(2)	117.37(3)	118.47(4)	119.77(3)	119.84(3)
Co-As-Co (°)	73.96 (2)	73.94 (3)	74.56(2)	74.33(3)	74.83 (3)	75.42 (2)	75.45 (3)
Diffractometer	PANalyitical X'Pert Pro						
Radiation type	Co Kα						
Wavelength (Å)	1.79026						
Collection Range (° 2θ)	10 to 130						
Step size (° 2θ)	0.017						
Number of Observations (*N*)	7059	7059	7059	7059	7059	7059	7059
Number of structure parameters (*P1*)	4	4	4	4	4	4	4
Number of profile parameters (*P2*)	9	9	9	9	9	9	9

R_p	3.87%	3.91%	3.34%	3.76%	4.15%	3.15%	2.25%
R_{wp}	5.46%	5.79%	4.62%	5.07%	5.69%	4.23%	2.91%
R_{exp}	1.67%	1.69%	1.76%	1.96%	1.81%	2.04%	1.42%
χ^2	10.7	11.7	6.91	6.68	9.87	4.65	4.19

Note: $R_p=\sum|y_{io}-y_{ic}|/\sum|y_{io}|$, $R_{wp}=[\sum w_i(y_{io}-y_{ic})^2/\sum w_i y_{io}^2]^{1/2}$, $R_{exp}=[\ (N-P_1-P_2)/\sum w_i y_{io}^2]^{1/2}$,

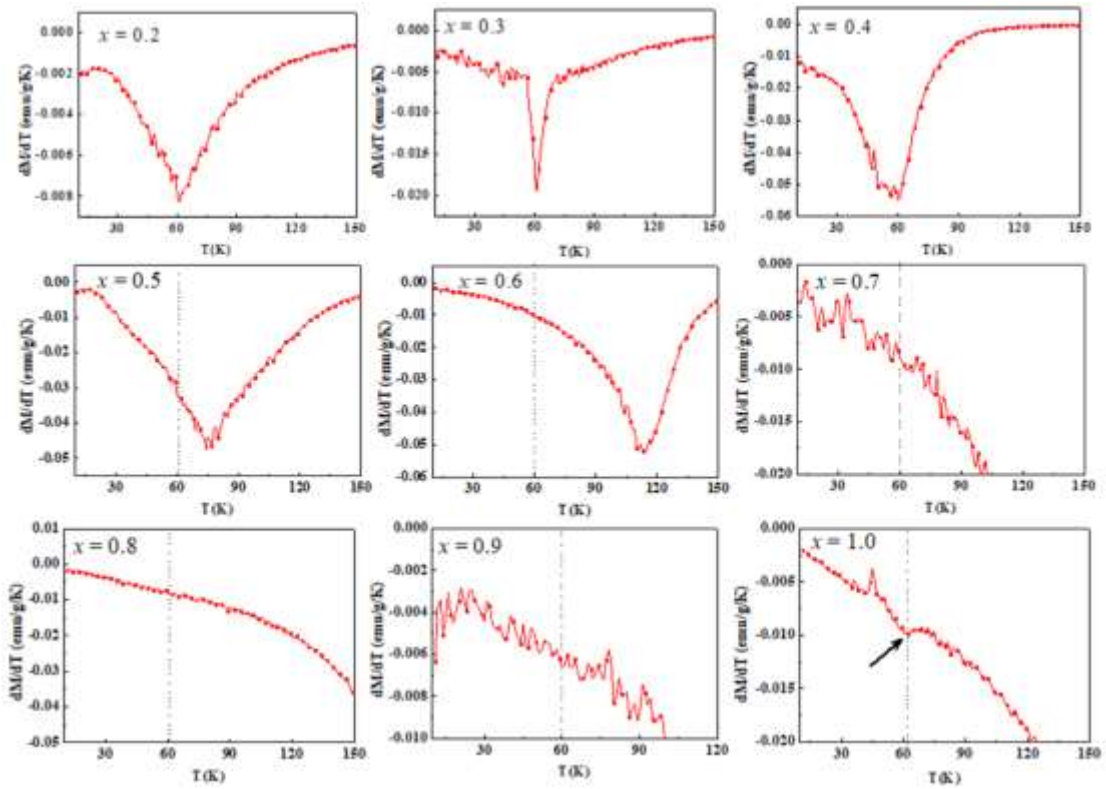

Fig.S1. The differential susceptibility of $Sr_{1-x}La_xCo_2As_2$ (nominal x = 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0). The magnetic signal of LaCoOAs is indicated by an arrow.