Electronic Supplementary Information for "Structural and electronic response upon hole doping of rare-earth iron oxyarsenides $Nd_{1-x}Sr_xFeAsO$ ($0 < x \leq 0.2$)"

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Table S1. Refined structural parameters and selected bond lengths (Å) and angles (°) for $Nd_{1-x}Sr_xFeAsO$ with x = 0.05, 0.1 and 0.2 obtained from Rietveld refinements of the synchrotron X-ray diffraction data at room temperature.

		$x = 0$	$x = 0.05$	$x = 0.1$	$x = 0.2$
Space group		*P4/nnm*	*P4/nnm*	*P4/nnm*	*P4/nnm*
a (Å)		3.96830(1)	3.971708(2)	3.97334(2)	3.97773(2)
c (Å)		8.60429(6)	8.57316(6)	8.58077(6)	8.64147(8)
Volume (Å^3)		135.495(1)	135.237(1)	135.469(1)	136.728(1)
Nd	B_{iso} (Å^2)	0.62(2)	0.39(1)	0.326(7)	0.45(2)
	Occ.	0.996(1)	0.944(6)	0.909(6)	0.79(1)
	z	0.13912(8)	0.13927(6)	0.13877(5)	0.13719(9)
Sr	B_{iso} (Å^2)		0.39(1)	0.326(7)	0.45(2)
	Occ.		0.052(6)	0.091(6)	0.21(1)
	z.		0.13927(6)	0.13877(5)	0.13719(9)
O	B_{iso} (Å^2)	2.0(3)	1.0(3)	0.6(1)	1.1(2)
	Occ	1.02(1)	1.00	1.00	1.00
Fe	B_{iso} (Å^2)	0.63(5)	0.53(3)	0.41(4)	0.47(5)
	Occ.	1.013(3)	1.00	1.00	1.00
As	B_{iso} (Å^2)	0.66(3)	0.52(1)	0.42(1)	0.46(3)
	Occ	1.023(2)	1.00	1.00	1.00
	z	0.6571(1)	0.6572(1)	0.6568(1)	0.6563(2)
R_{wp} (%)		5.27	6.50	6.71	6.42
R_{exp} (%)		3.37	3.80	4.34	4.11
Nd-O (Å)		2.3173(4) x 4	2.3171(3) x 4	2.3162(2) x 4	2.3151(4) x 4
Fe-Fe (Å)		2.80601(1) x 4	2.80842(1) x 4	2.80958(1) x 4	2.81268(1) x 4
Fe-As(Å)		2.4010(7) x 4	2.3998(5) x 4	2.3994(4) x 4	2.4045(5) x 4
Fe-As-Fe (Å)		111.46(5) x 2 71.51(2) x 4	111.69(1) x 2 71.63(2) x 4	111.79(4) x 2 71.67(2) x 4	111.62(4) x 2 71.59(2) x 4

P4/nmm: Nd/Sr on 2*c* (¼, ¼, *z*), Fe on 2*b* (¾, ¼, ½), O on 2*a* (¾, ¼, 0), As on 2*c* (¼, ¼, *z*).

Figure S1. Final observed (circles) and calculated (solid lines) synchrotron X-ray (λ = 0.40301 Å) powder diffraction profiles for $Nd_{1-x}Sr_xFeAsO$ with x = 0, 0.05, 0.1 and 0.2 at room temperature. The lower solid lines show the difference profiles and the tick marks show the reflection positions. The high resolution/high statistics data were collected in the 2θ range between 2 and 50º. Here only part of the diffraction profiles is shown for clarity.

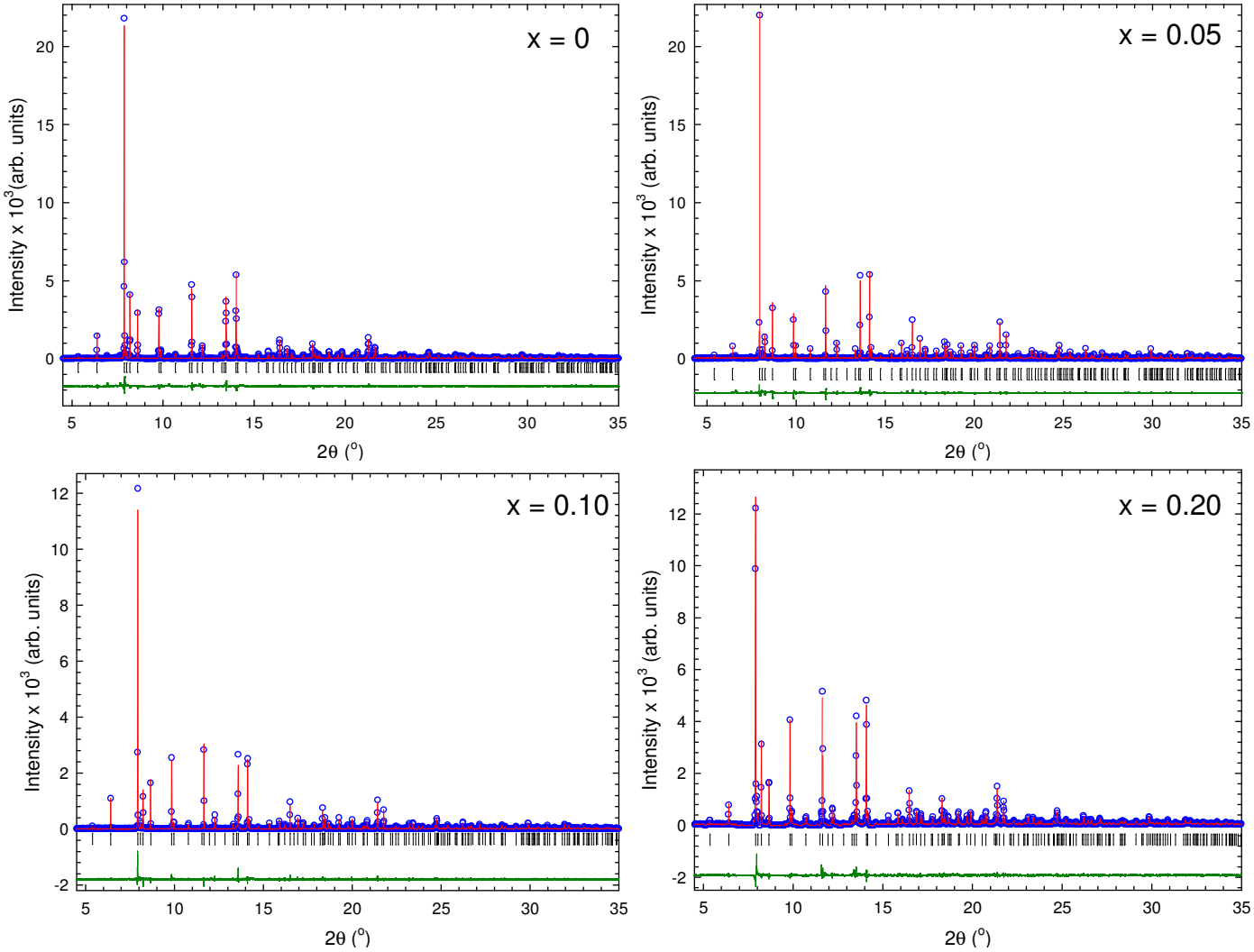

Figure S2. Evolution of selected distances and angles as a function of doping level *x* in $Nd_{1-x}Sr_xFeAsO$. The red and green circles refer to the data at room temperature and 5 K respectively. The structural phase transition from tetragonal-to-orthorhombic results in the splitting of the Fe-Fe distances and of the Fe-As-Fe angles. High statistics data for the parent compound NdFeAsO were collected only at room temperature.

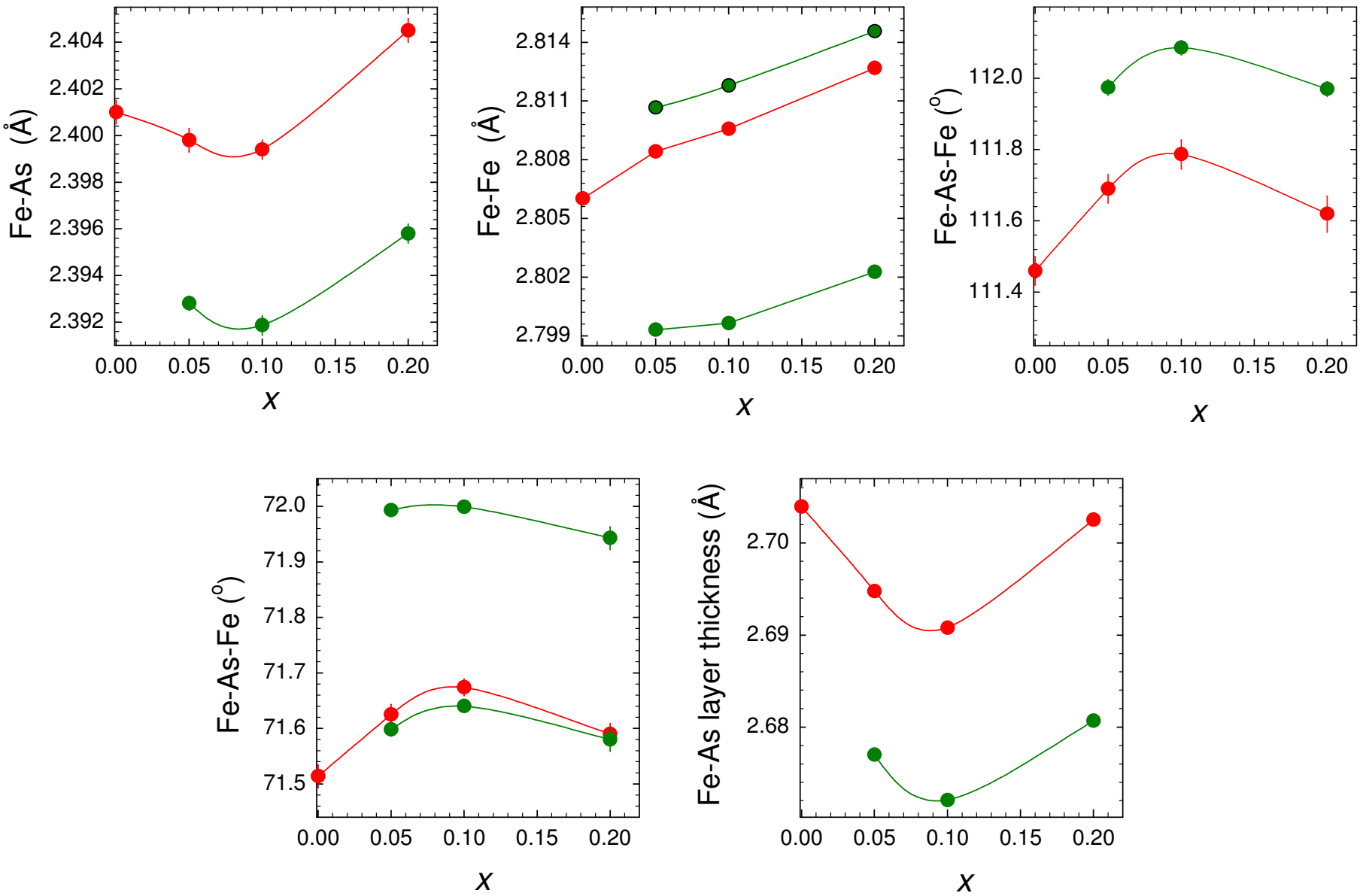

Table S2. Refined structural parameters and selected bond lengths (Å) and angles (°) for $Nd_{1-x}Sr_xFeAsO$ with x = 0.05, 0.1 and 0.2 obtained from Rietveld refinements of the synchrotron X-ray diffraction data at 5 K. High statistics data for the parent compound NdFeAsO were collected only at room temperature.

		$x = 0.05$	$x = 0.1$	$x = 0.2$
Space group		*Cmma*	*Cmma*	*Cmma*
a (Å)		5.59862(1)	5.59930(2)	5.60451(2)
b (Å)		5.62133(1)	5.62358(1)	5.62914(1)
c (Å)		8.53437(2)	8.54437(2)	8.60519(2)
Volume (Å^3)		268.591(1)	269.046(1)	271.482(1)
Nd	B_{iso} (Å^2)	0.038(4)	0.041(3)	0.10(1)
	Occ.	0.952(5)	0.906(6)	0.805(4)
	z	0.1395(4)	0.13924(3)	0.13842(3)
Sr	B_{iso} (Å^2)	0.038(4)	0.041(3)	0.10(1)
	Occ.	0.048(5)	0.094(3)	0.195(4)
	z.	0.1395(4)	0.13924(3)	0.13842(9)
O	B_{iso} (Å^2)	0.23(6)	0.26(5)	0.8(3)
	Occ	1.00	1.00	1.00
Fe	B_{iso} (Å^2)	0.026(4)	0.014(3)	0.098(4)
	Occ.	1.00	1.00	1.00
As	B_{iso} (Å^2)	0.020(3)	0.030(3)	0.09(3)
	Occ	1.00	1.00	1.00
	z	0.65684(6)	0.65470(5)	0.65576(8)
R_{wp} (%)		5.25	5.87	4.99
R_{exp} (%)		3.04	3.85	3.29
Nd-O (Å)		2.3135(2) x 4	2.3131(4) x 4	2.3157(2) x 4
Fe-Fe (Å)		2.81066(1) x 2 2.79931(1) x 2	2.81179(1) x 2 2.79965(1) x 2	2.81456(1) x 4 2.80227(1) x 2
Fe-As(Å)		2.3928(3) x 4	2.3919(4) x 4	2.3958(4) x 4
Fe-As-Fe (Å)		111.97(2) x 2 71.60(1) x 2 71.99(1) x 2	112.09(2) x 2 71.64(1) x 2 72.00(2) x 2	111.97(2) x 2 71.58(2) x 2 71.94(2) x 2

Cmma: Nd/Sr on 4*g* (0, ¼, *z*), Fe on 4*b* (¼, 0, ½), O on 4*a* (¼, 0, 0), As on 4*g* (0, ¼, *z*).

Figure S3. Evolution of the normalised volume, of the Fe-As distance and of the Fe-As-Fe angle as a function of temperature for $Nd_{1-x}Sr_xFeAsO$. The green, blue and red circles refer to x =0.05, 0.1 and 0.2, respectively.