Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

In situ study of copper reduction in $SrTi_{1-x}Cu_xO_3$ nanoparticles

Supporting Information

Contents

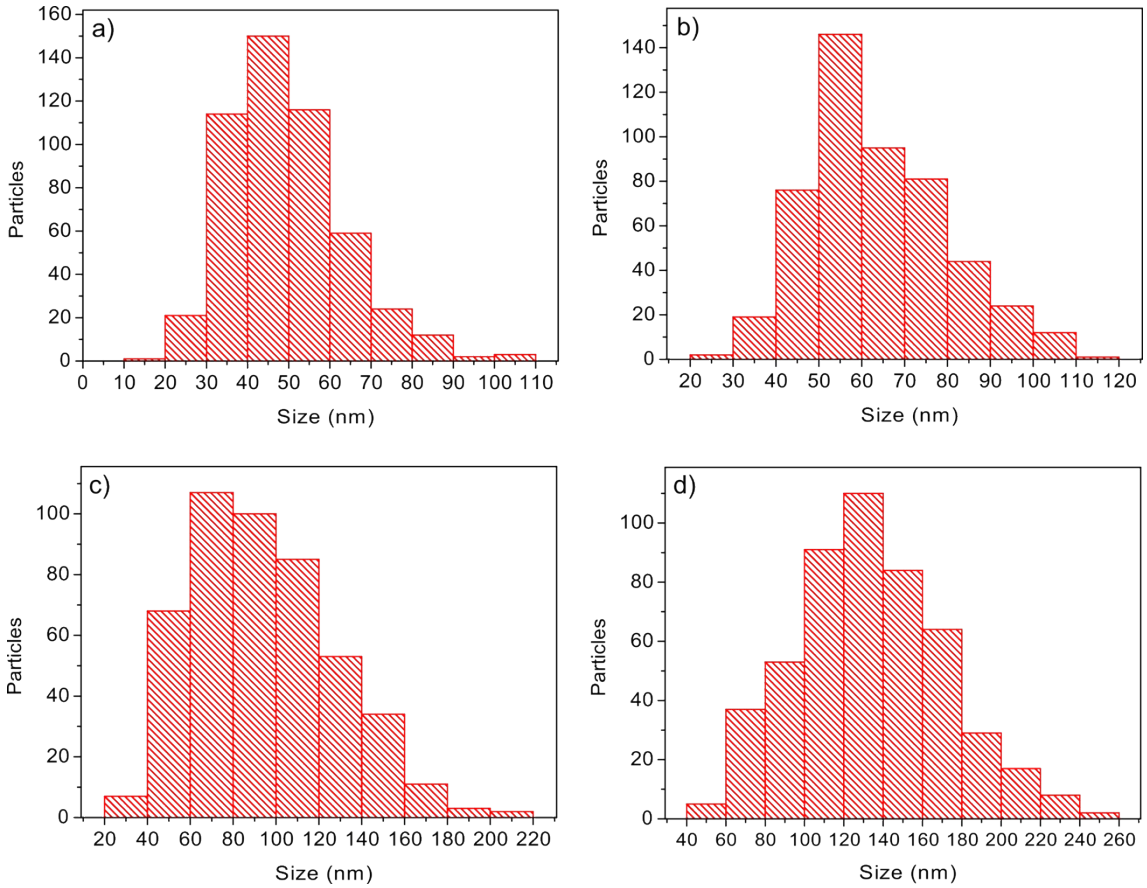

Figure S1 – Particle size distribution for the x = 0.00 (a), 0.03 (b), 0.09 (c) and 0.15 (d) samples from scanning electron microscopy images.

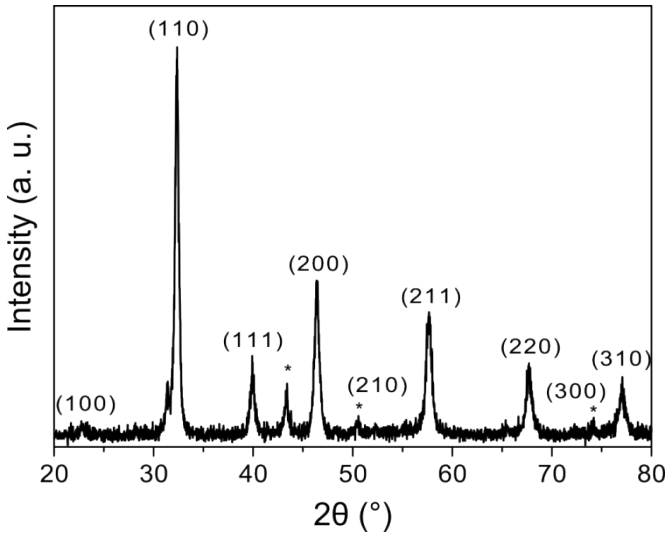

Figure S2 – X-ray diffraction pattern of $SrTi_{0.85}Cu_{0.15}O_3$ sample after reduction at 1100 K for 30 min. Indexes are attributed to $SrTiO_3$ phase. * represents Cu phase. The two-theta range was scanned continuously at 2°/min.

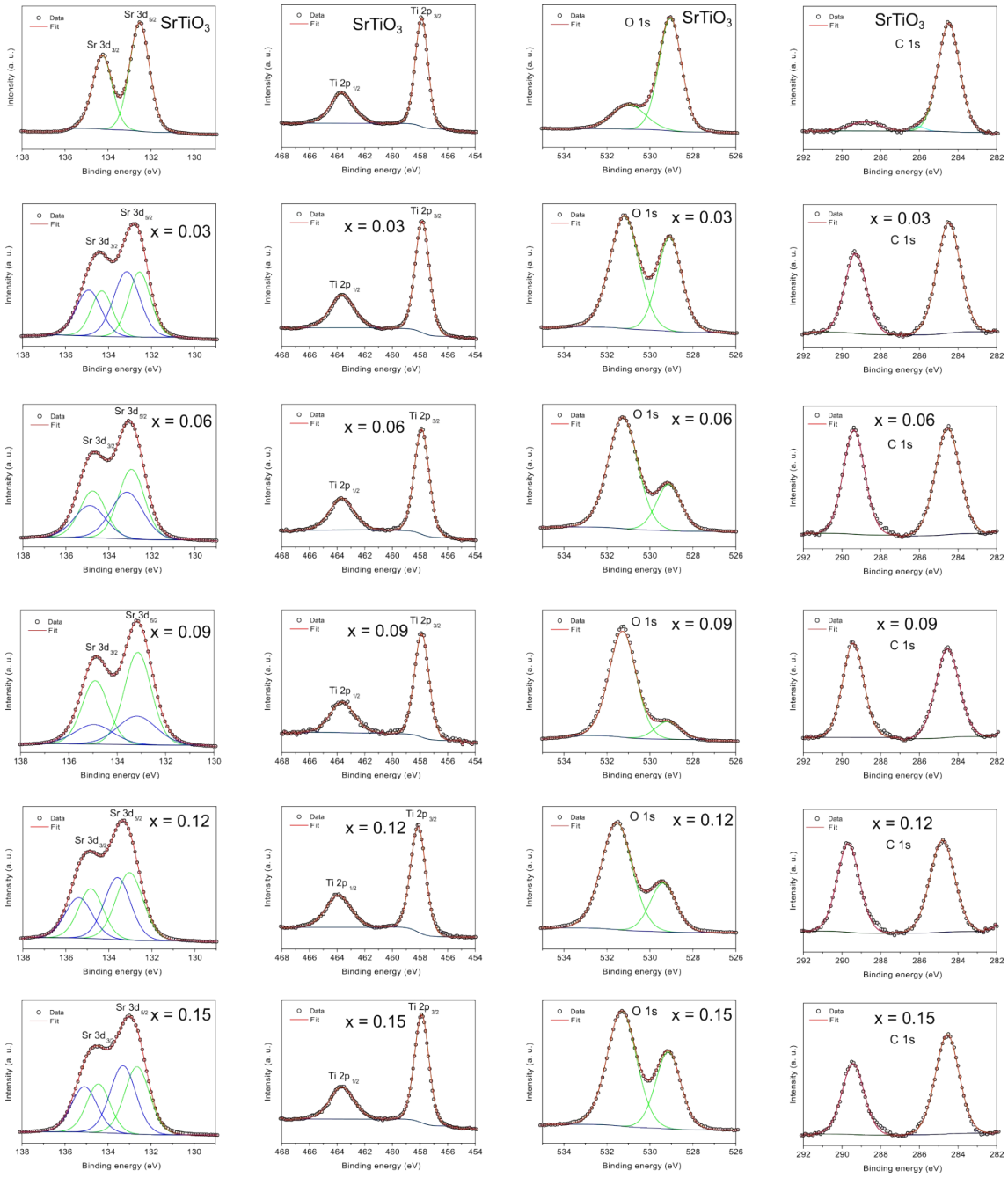

Figure S3 – Room temperature XPS spectra of $SrTi_{1-x}Cu_xO_3$ samples in the regions of Sr 3d, Ti 2p, O 1s and C 1s peaks. Blue and green components in Sr 3d region represent Sr in $SrCO_3$ and in $SrTiO_3$, respectively.

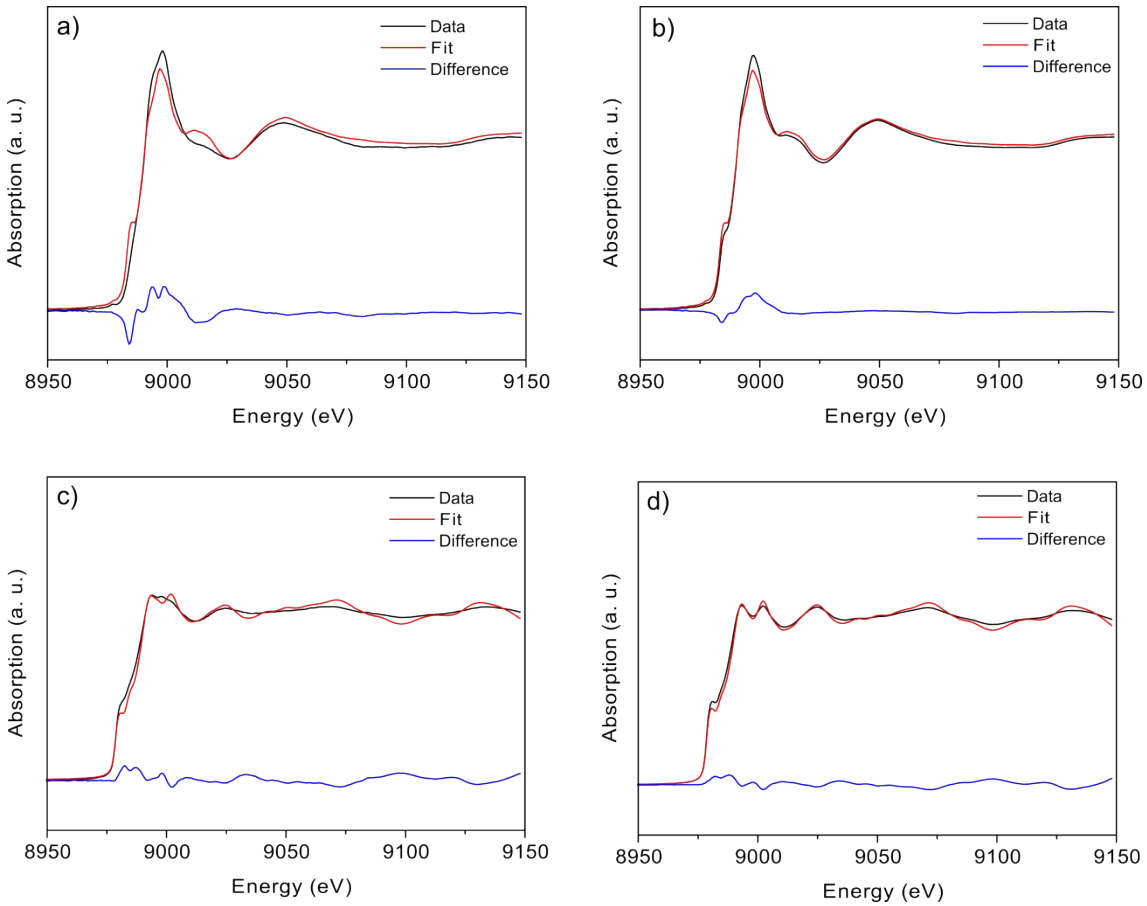

Figure S4 – Least-square linear combination fits: (a) x = 0.03 and (b) x = 0.15 samples measured at room temperature under an ambient atmosphere; (c) x = 0.03 and (d) x=0.15 samples measured at 550 K in hydrogen-rich atmosphere.

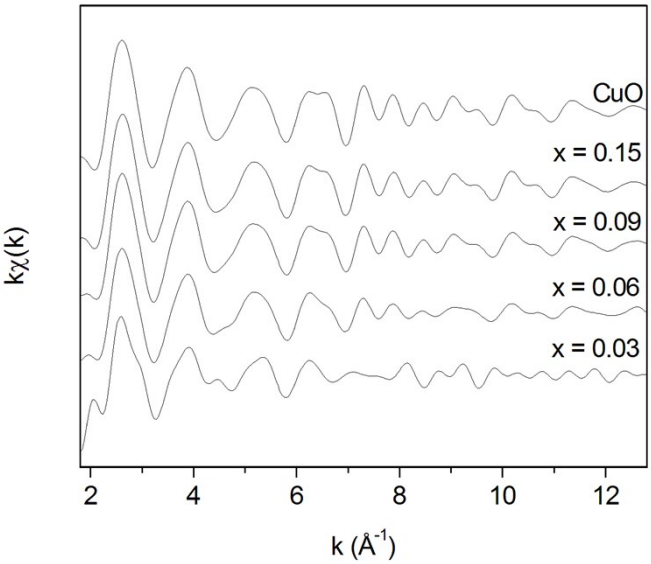

Figure S5 - Filtered inverse Fourier transform EXAFS spectra of samples measured at room temperature under an ambient atmosphere considering the interval between 2.07 and 6.5 Å. CuO data is shown for comparison.

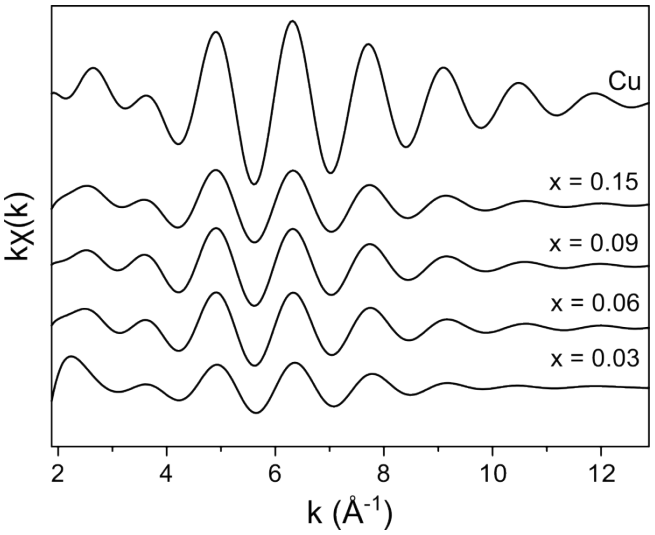

Figure S6 – Filtered inverse Fourier transform EXAFS spectra of the samples measured at 550 K in hydrogen-rich atmosphere considering the interval between 1.38 and 2.84 Å. Cu data is shown for comparison.

	Linear Combination		
	C(Cu) %	C(CuO)%	QF
x=0.03 oxidized	0	100	14
x=0.03 reduced	77(1)	23(1)	4
x=0.06 oxidized	0	100	8
x=0.06 reduced	89(1)	11(1)	2
x=0.09 oxidized	0	100	6
x=0.09 reduced	92(1)	8(1)	3
x=0.15 oxidized	0	100	5
x=0.15 reduced	92(1)	8(1)	3

Table S1- Linear combination results of the XANES experimental spectra using the two standards samples, Cu metal and CuO. C = percentage of CuO and Cu phases and QF = Fitting Quality factor .Errors are given in parenthesis. Oxidized: measured at room temperature under ambient atmosphere; reduced: measured in a hydrogen-rich atmosphere after reaching 550 K.