Structural and Catalytic Effects of Iron- and Scandium-Doping on a Strontium Cobalt Oxide Electrocatalyst for Water Oxidation

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XRD Data of SCO Precursors

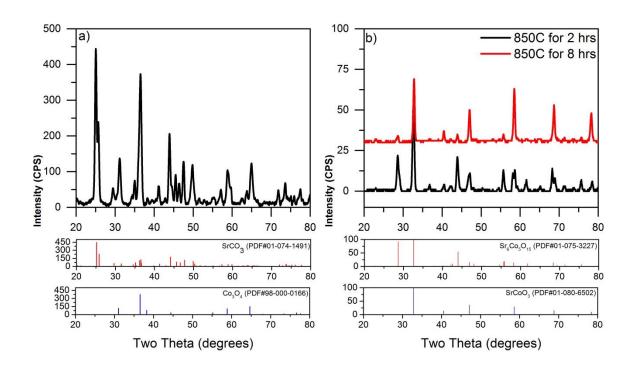


Figure S1. XRD spectra of a) SCO precursor annealed for 4.5 hours at 450°C, b) SCO precursor annealed at 850°C for 2 and 8 hours

XPS Data of All SCO Samples

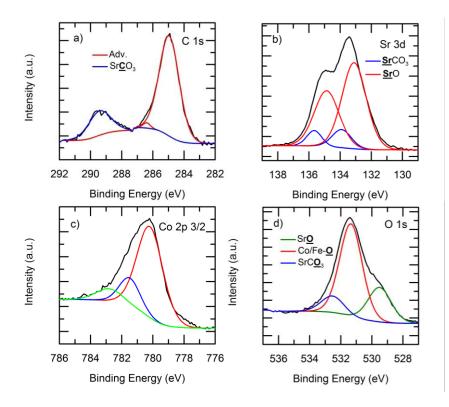


Figure S2. XPS spectra and fitted peaks for the 1%Fe-SCO sample. a) Spectra of the carbon 1s peak. b) Spectra of the strontium 3d 5/2 and 3/2 peaks. c) Spectra of the cobalt 2p peak. d) Spectra of the oxygen 1s peak.

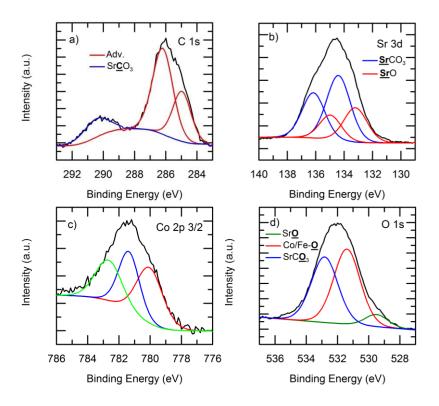


Figure S3. XPS spectra and fitted peaks for the 5% Fe-SCO sample. a) Spectra of the carbon 1s peak. b) Spectra of the strontium 3d 5/2 and 3/2 peaks. c) Spectra of the cobalt 2p peak. d) Spectra of the oxygen 1s peak.

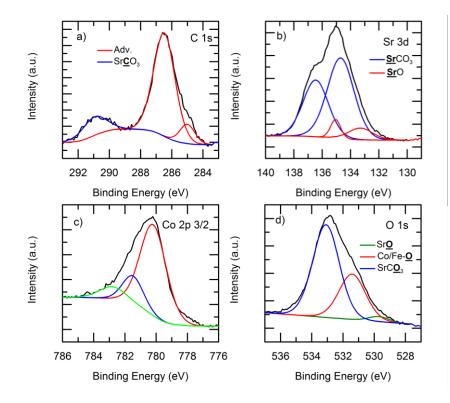


Figure S4. XPS spectra and fitted peaks for the 1%Sc-SCO sample. a) Spectra of the carbon 1s peak. b) Spectra of the strontium 3d 5/2 and 3/2 peaks. c) Spectra of the cobalt 2p peak. d) Spectra of the oxygen 1s peak.

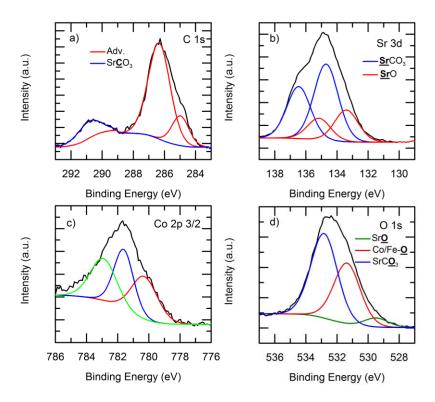


Figure S5. XPS spectra and fitted peaks for the 5%Sc-SCO sample. a) Spectra of the carbon 1s peak. b) Spectra of the strontium 3d 5/2 and 3/2 peaks. c) Spectra of the cobalt 2p peak. d) Spectra of the oxygen 1s peak.

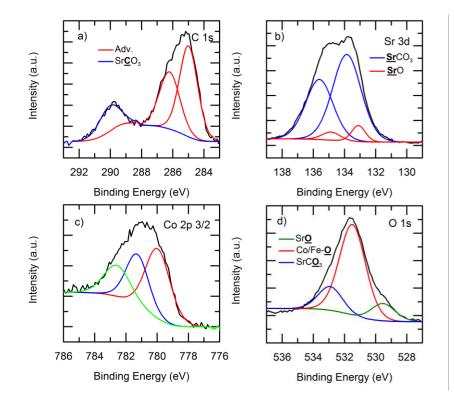


Figure S6. XPS spectra and fitted peaks for the 10%Sc-SCO sample. a) Spectra of the carbon 1s peak. b) Spectra of the strontium 3d 5/2 and 3/2 peaks. c) Spectra of the cobalt 2p peak. d) Spectra of the oxygen 1s peak.

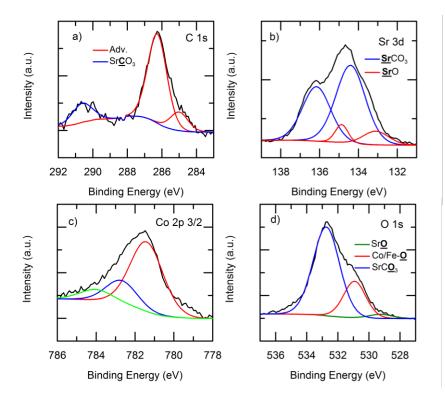


Figure S7. XPS spectra and fitted peaks for the UnSCO sample. a) Spectra of the carbon 1s peak. b) Spectra of the strontium 3d 5/2 and 3/2 peaks. c) Spectra of the cobalt 2p peak. d) Spectra of the oxygen 1s peak.

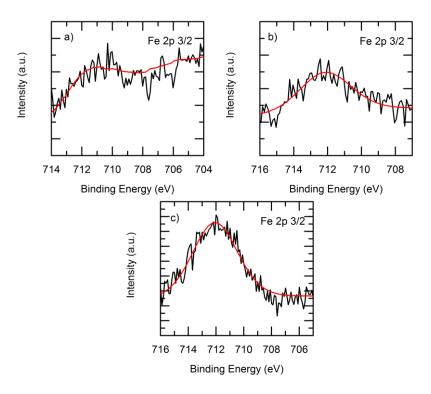


Figure S8. XPS spectra and fitted peaks for the Fe 2p 3/2 peaks of the Fe-SCO samples. a) 1%Fe-SCO b) 5%Fe-SCO c) 10%Fe-SCO

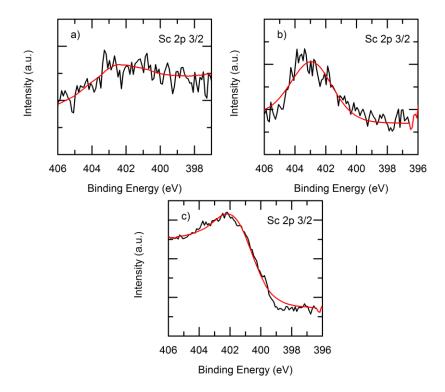


Figure S9. XPS spectra and fitted peaks for the Sc 2p 3/2 peaks of the Sc-SCO samples. a) 1%Sc-SCO b) 5%Sc-SCO c) 10%Sc-SCO

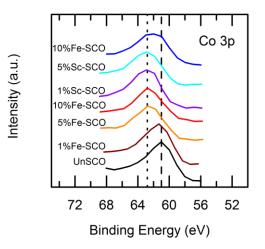


Figure S10. XPS spectra of the Co 3p region in all SCO samples. The dashed line lies on 61.0 eV, the dotted line lies on 62.8 eV

TEM Figures of SCO Powders

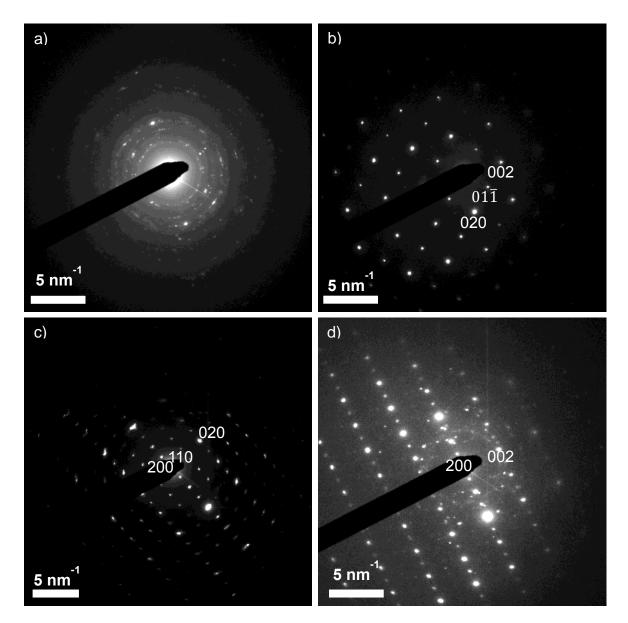


Figure S11. Selected area electron diffraction patterns of a) UnSCO, b) 5%Fe-SCO, c) 10%Fe-SCO), and d) 10% Sc-SCO showing the polycrystalline nature of the undoped material. The other diffraction patterns have been indexed as orthorhombic SrCoO_{2.5}.

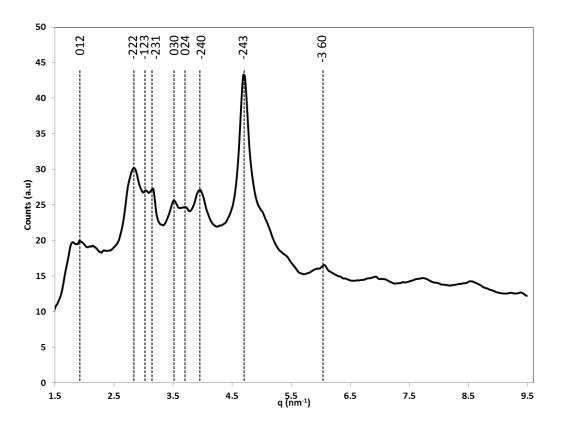


Figure S12. Radial distribution plot of the SAED in Figure SX1 for UnSCO integrated over 360° indexed as trigonal $Sr_6Co_5O_{15}$.

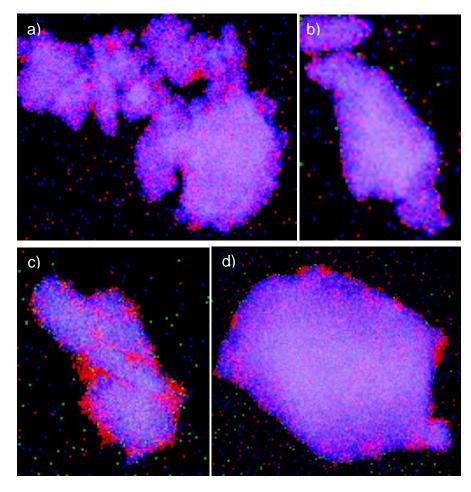


Figure S13. Electron dispersive X-ray spectroscopy maps of a) UnSCO, b) 5%Fe-SCO, c) 10%Fe-SCO, and d) 10% Sc-SCO. Cobalt is blue, strontium is red, and the dopant (Fe or Sc) is green.

SEM Figures of All SCO Electrodes

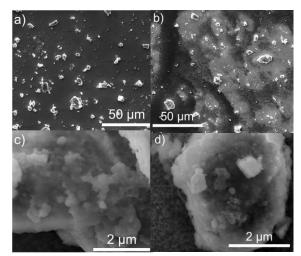


Figure S14. SEM images of a) 10%Fe-SCO and b) undoped SCO microparticle catalyst on conductive FTO substrate. Surface morphology for the c) 10%Fe-SCO and d) undoped SCO microparticles both appear rough, and composed of sintered microparticles.

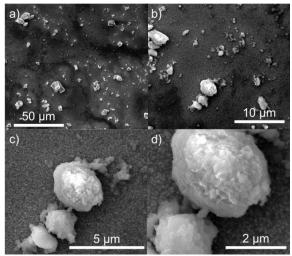


Figure S16. SEM images of 1% Fe-SCO Electrode

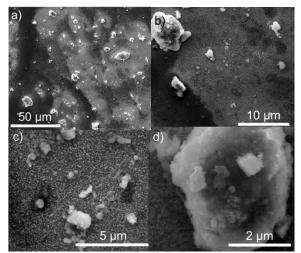


Figure S15. SEM images of UnSCO Electrode

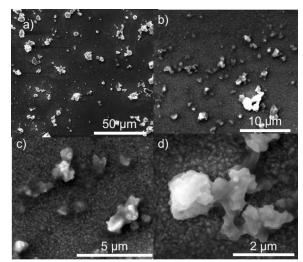


Figure S17. SEM images of 5% Fe-SCO Electrode

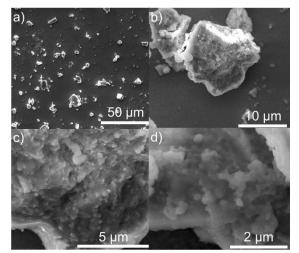


Figure S18. SEM images of 10% Fe-SCO Electrode

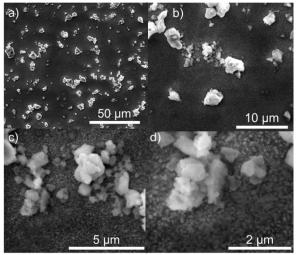


Figure S20. SEM images of 5% Sc-SCO Electrode

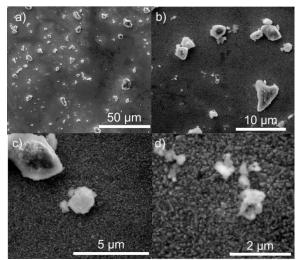


Figure S19. SEM images of 1%Sc-SCO Electrode

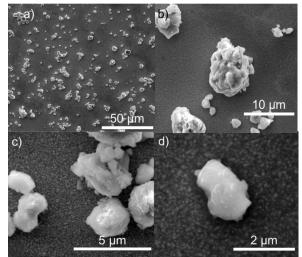


Figure S21. SEM images of 10% Sc-SCO Electrode

OER Performance

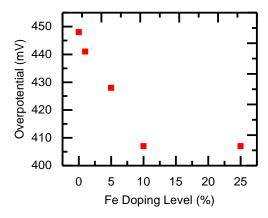


Figure S22. Plot of measured overpotential at 10 mA/cm² versus [Fe] in several Fe-doped SCO electrodes

Supporting Tables

Table S1: Tolerance values for the seven selected SCO samples examined in this study. *t* shows a transition to unity with increasing concentrations of both Fe and Sc dopants.

t
1.002
1.002
1.001
1.000
1.001
0.996
0.989

Table S2: Atomic percentage of Fe and Sc dopants as measured using XPS, and the binding energy of the 2p 3/2 peaks both elements.

Sample	Percent Fe/Sc (%)	Binding Energy (eV)
1%Fe-SCO	1.14	711.9
5%Fe-SCO	3.78	712.2
10%Fe-SCO	9.10	712.9
1%Sc-SCO	3.95	402.7
5%Sc-SCO	5.18	402.9
10%Sc-SCO	13.61	401.6

Table S3: FWHM and Co 2p 3/2 binding energies for the Fe-SCO samples. As iron concentration increases, the FWHM of the peak increases as well.

Sample	Binding Energy (eV)	FWHM
1%Fe-SCO	780.2	2.49
5%Fe-SCO	781.5	3.20
10%Fe-SCO	781.2	3.37

Table S4: OER mass activities of several perovskites. LaNiO₃, LaNi_{0.75}Fe_{0.25}O₃, LaCoO₃, and LaMnO₃ are all supported on N-doped carbon on a glassy carbon rotating disk electrode.

	Mass
Sample	Activity
	(mA/mg)
SrCo _{0.9} Fe _{0.1} O _{3-δ}	6.5
LaNiO ₃ *	90.0
LaNi _{0.75} Fe _{0.25} O ₃ *	82.0
LaCoO ₃ *	100.0
LaMnO ₃ *	92

*Adapted from Reference 51