Synthesis and Characterization of $Sr_2Co_{2-x}Fe_xO_{5+d}$ Perovskite Oxides

Sivasankara Rao Ede[1], Carlos Poasada[1], Jessa Guffie[1], William Ratcliff[2], Hui Wu[2], Shubo Han[1] and Zhiping Luo[1]

[1]Fayetteville State University, FAYETTEVILLE, North Carolina, United States, [2]National Institute of Standards and Technology, Gaithersburg, Maryland, United States

In the past few decades, the overwhelming use of conventional fuels in automobiles and industries has hampered the environment severely, due to the generation of pollutions. In order to mitigate these pollution-related issues, research communities have sought the production of fuels in a "greener" and environmentally conscientious manner. Amid these technologies, electrochemical water splitting, which produces oxygen and hydrogen for fuel cells to further make electricity, shows potentials.1 The main challenge in improving the energy efficiency of water electrolysis is the sluggish kinetics associated with oxygen evolution reaction (OER). Currently, several OER catalysts have been found to improve the efficiency of this reaction, including RuO_2 and IrO_2 catalysts. Unfortunately, the high cost and scarcity of Ru and Ir have hindered the use of these materials on an industrial scale. Alternatively, transition metal oxides like Co, Ni, and Fe have also shown excellent energy efficiency. Octahedrally coordinated Co-based oxide materials, such as perovskites and spinel oxides, have shown especially enhanced OER activity.2 Perovskite oxides are well known for having the general formula of ABO_3 and exhibit excellent physical, chemical, and catalytic properties.3 Rare earth metals, alkaline earth metals, or p-block elements are often incorporated at the A-site. In contrast, transition elements generally occupy the B-site. $LaCoO_3$ was the first reported perovskite oxide to be used as a catalyst for OER4 and since then, numerous perovskite oxides have been reported as electrocatalysts for OER.5 In this work, $Sr_2Co_{2-x}Fe_xO_{5+d}$ oxides were synthesized, and their crystalline, magnetic, and electrochemical water-oxidation properties were studied. It was observed that by changing the elemental ratio between Co and Fe ($Sr_2Co_2O_{5+\delta}$, $Sr_2Co_{1.75}Fe_{0.25}O_{5+\delta}$, $Sr_2Co_{1.5}Fe_{0.5}O_{5+\delta}$, $Sr_2Co_{1.25}Fe_{0.75}O_{5+\delta}$, $Sr_2CoFeO_{5+\delta}$, $Sr_2Co_{0.75}Fe_{1.25}O_{5+\delta}$, $Sr_2Co_{0.5}Fe_{1.5}O_{5+\delta}$, $Sr_2Co_{0.25}Fe_{1.75}O_{5+\delta}$ and $Sr_2Fe_2O_{5+\delta}$) the magnetic and electrochemical behavior of the material was considerably affected. Hence, we intend to correlate structural, electrochemical, and magnetic properties of the material with the help of neutron diffraction studies using BT-1 instrumentation in the temperature range of 5-350 K. SEM analysis demonstrates that all samples exhibit irregular microstructures composed of small nanoparticles (Figure 1a and b). The EDS spectra of $Sr_2Co_2O_{5+\delta}$, $Sr_2Co_{1.5}Fe_{0.5}O_{5+\delta}$, $Sr_2CoFeO_{5+\delta}$, $Sr_2Co_{0.5}Fe_{1.5}O_{5+\delta}$ and $Sr_2Fe_2O_{5+\delta}$ are displayed in Figure 2. All spectra are normalized with the Sr $L\alpha$ peak (1.806 keV). The magnified region in 6-8 keV is shown at the right side of the figure, exhibiting the intensity variations of Fe $K\alpha/K\beta$ peaks (6.398/7.056 keV) Co $K\alpha/K\beta$ peaks (6.923/7.647 keV). According to Shao-Horn's principle, a rationally designed OER catalyst ought to have an eg filling value approaching 1.2, therefore, the synthesized oxides were manufactured with this mindset.6 Concurrently, the OER activity of $Sr_2Co_{1.5}Fe_{0.5}O_{5+\delta}$ was the most efficient. We conducted neutron scattering for the magnetic structures correlating with magnetic data.7
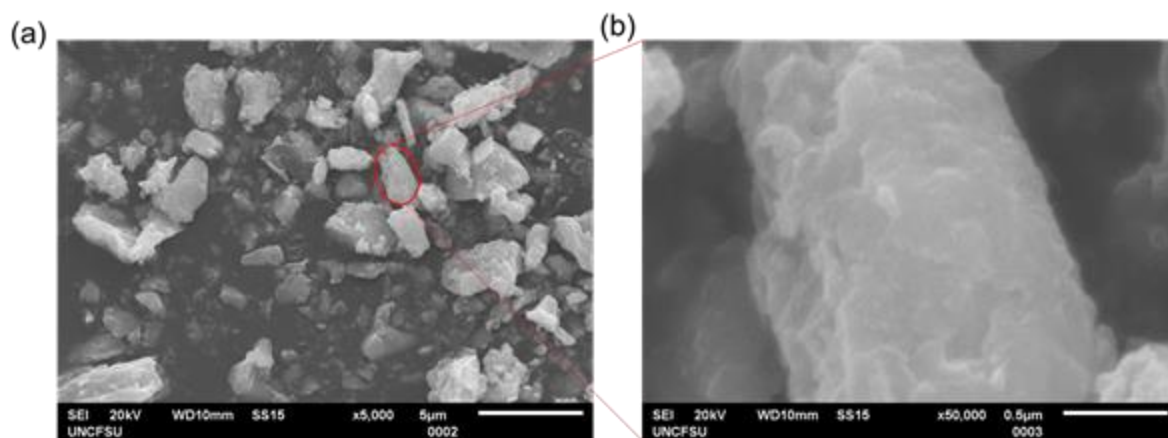
Figure 1. Figure 1. SEM images of representative Sr2Co2-xFexO5+δ oxide powders at low magnification (a) and high magnificatiion (b).
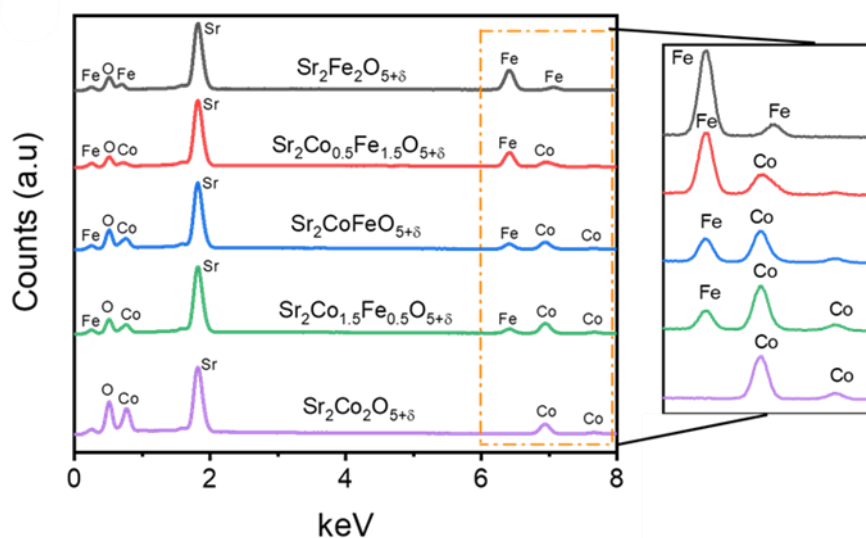
Figure 2. Figure 2. (a) EDS spectra of Fe/Co of the representative Sr2Co2-xFexO5+δ oxides.

References

1. Gür, T. M. *Energy Environ. Sci.* **2018**, *11*, 2696.

2. Jin, H.; Wang, J.; Su, D.; Wei, Z.; Pang, Z.; Wang, Y. *Am. Chem. Soc.* **2015**, *137*, 2688.

3. George, G. et al. *Int.* **2018**, *44*, 21982.

4. G. Hardin, J. T. Mefford, D. A. Slanac, B. B. Patel, X. Wang, S. Dai, X. Zhao, R. S. Ruoff,

5. P. Johnston and K. J. Stevenson, *Chem. Mater.,* **2014,** *26*, 3368.

6. Yin, W.-J.; Weng, B.; Ge, J.; Sun, Q.; Li, Z.; Yan, Y. *Energy Environ. Sci.,* **2019**,*12*, 442.

7. Suntivich, J., May, K. J., Gasteiger, H. A., Goodenough, J. B. & Shao-Horn, Y. *Science* **2011,** *334*, 1383.