

## Supplementary Information

### **Boosting the oxygen evolution activity in non-stoichiometric praseodymium ferrite-based perovskites by A site substitution for alkaline electrolyser anodes**

Steve Ward,<sup>a</sup> Mark A. Isaacs,<sup>b,c</sup> Gaurav Gupta,<sup>a</sup> Mohamed Mamlouk,<sup>a</sup> Stevin S. Pramana<sup>\*a</sup>

#### Affiliations

<sup>a</sup> School of Engineering, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK

<sup>b</sup> HarwellXPS, R92 Research Complex at Harwell, Rutherford Appleton Laboratories, Didcot, OX11 0QS, UK

<sup>c</sup> Department of Chemistry, University College London, London, WC1H 0AJ, UK

\* email: [stevin.pramana@newcastle.ac.uk](mailto:stevin.pramana@newcastle.ac.uk)

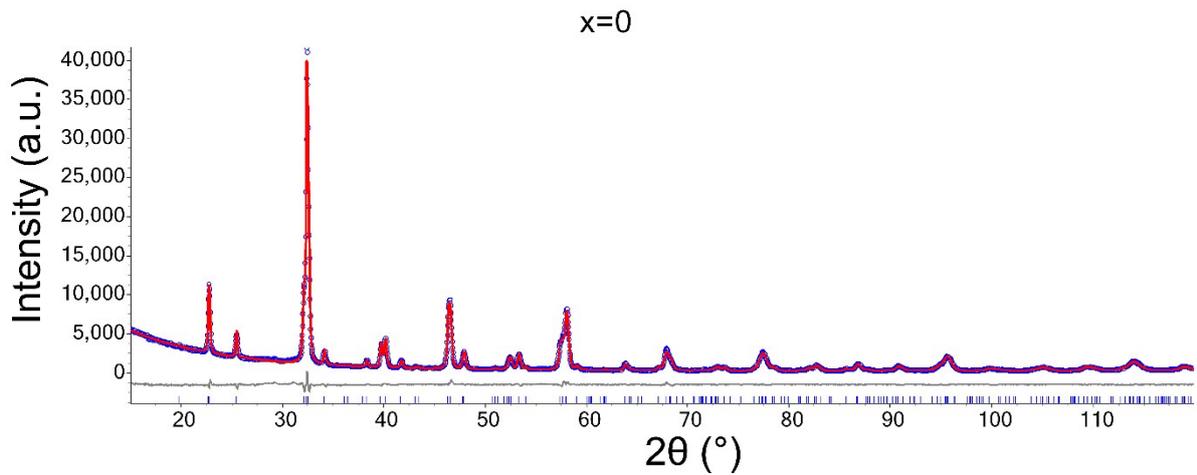


Figure S1 – Rietveld plot of the powder XRD data for  $\text{PrFeO}_{3-\delta}$  ( $x = 0$ ). This data was collected at room temperature and under ambient pressure. The observed intensity is shown in blue, the calculated intensity is shown in red, and the difference is shown in grey underneath. Vertical markers indicate Bragg reflections. ( $R_{\text{wp}} = 4.76\%$ ,  $R_{\text{Bragg}} = 1.55\%$ ).

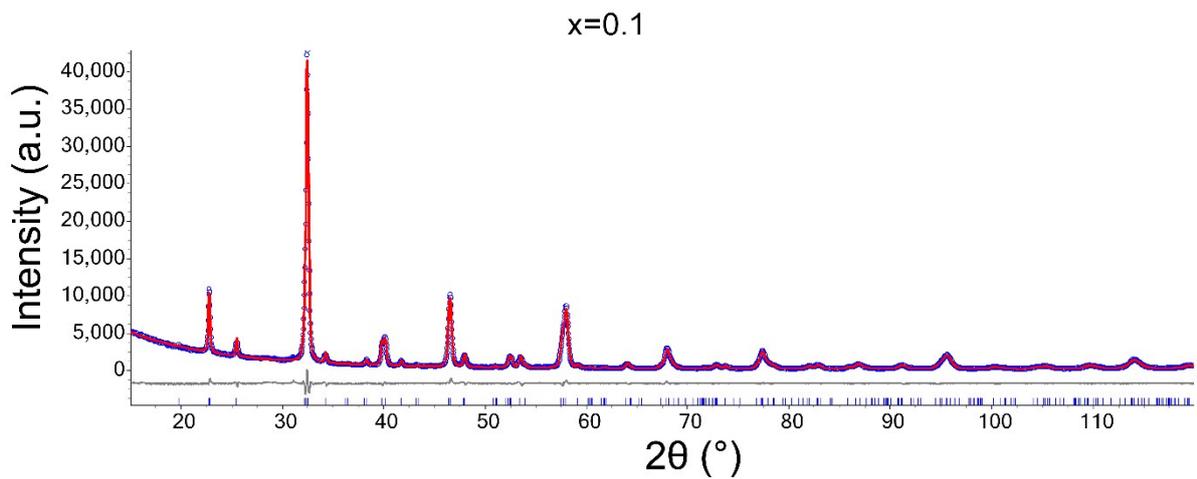


Figure S2 – Rietveld plot of the powder XRD data for  $\text{Pr}_{0.90}\text{Sr}_{0.10}\text{FeO}_{3-\delta}$  ( $x = 0.1$ ). This data was collected at room temperature and under ambient pressure. The observed intensity is shown in blue, the calculated intensity is shown in red, and the difference is shown in grey underneath. Vertical markers indicate Bragg reflections. ( $R_{\text{wp}} = 5.10\%$ ,  $R_{\text{Bragg}} = 1.57\%$ ).

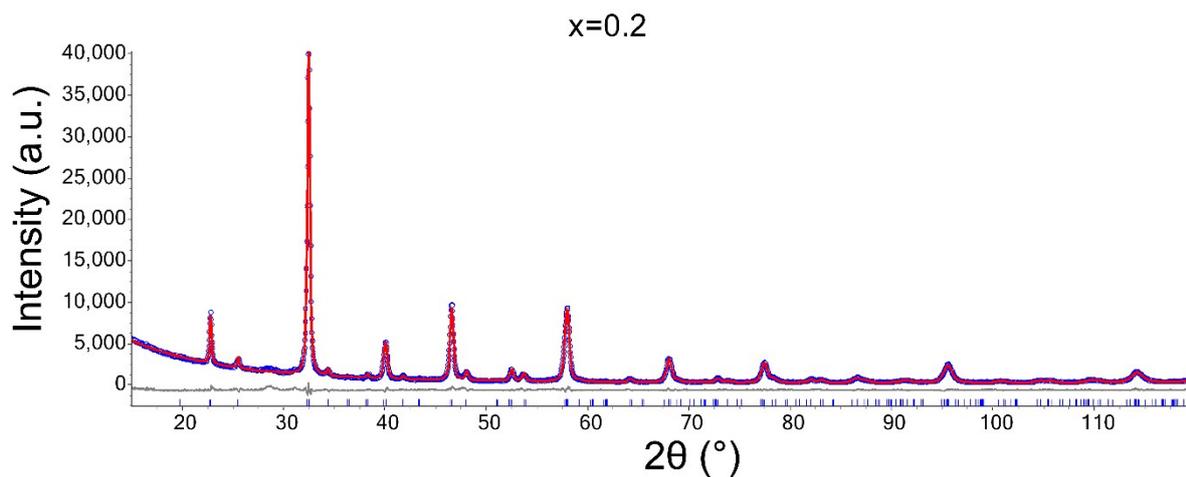


Figure S3 – Rietveld plot of the powder XRD data for  $\text{Pr}_{0.79}\text{Sr}_{0.21}\text{FeO}_{3-\delta}$  ( $x = 0.2$ ). This data was collected at room temperature and under ambient pressure. The observed intensity is shown in blue, the calculated intensity is shown in red, and the difference is shown in grey underneath. Vertical markers indicate Bragg reflections. ( $R_{\text{wp}} = 5.23\%$ ,  $R_{\text{Bragg}} = 1.18\%$ ).

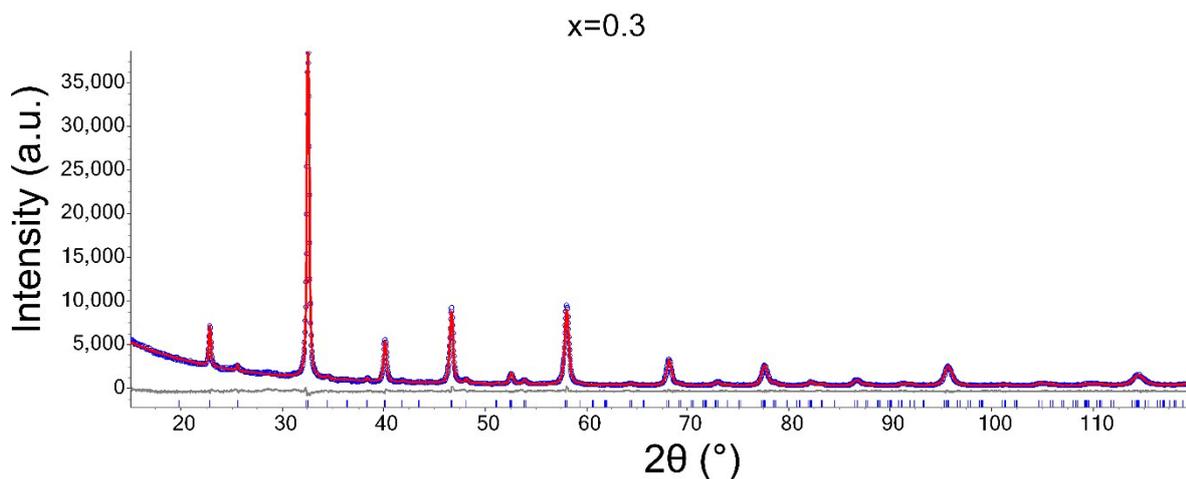


Figure S4 – Rietveld plot of the powder XRD data for  $\text{Pr}_{0.70}\text{Sr}_{0.30}\text{FeO}_{3-\delta}$  ( $x = 0.3$ ). This data was collected at room temperature and under ambient pressure. The observed intensity is shown in blue, the calculated intensity is shown in red, and the difference is shown in grey underneath. Vertical markers indicate Bragg reflections. ( $R_{\text{wp}} = 4.71\%$ ,  $R_{\text{Bragg}} = 1.31\%$ ).

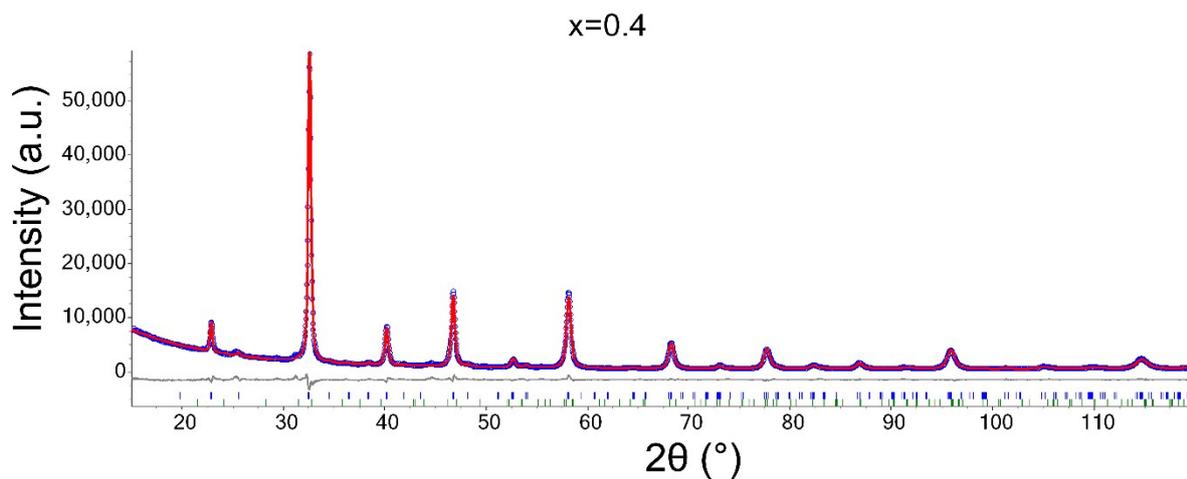


Figure S5 – Rietveld plot of the powder XRD data for  $\text{Pr}_{0.58}\text{Sr}_{0.42}\text{FeO}_{3-\delta}$  ( $x = 0.4$ ). This data was collected at room temperature and under ambient pressure. The observed intensity is shown in blue, the calculated intensity is shown in red, and the difference is shown in grey underneath. Vertical markers indicate Bragg reflections of 99.04(9) wt.% P6S4FO (top) and 0.96(9) wt.%  $\text{Pr}_2\text{FeO}_4$  (bottom) phases ( $R_{\text{wp}} = 5.23\%$ ,  $R_{\text{Bragg}} = 1.71\%$ ).

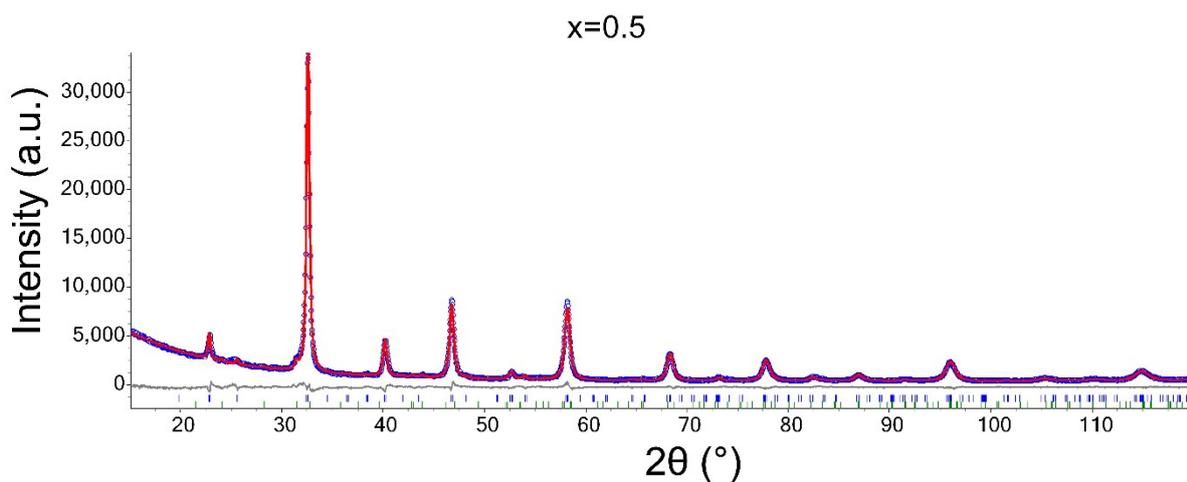


Figure S6 – Rietveld plot of the powder XRD data for  $\text{Pr}_{0.48}\text{Sr}_{0.52}\text{FeO}_{3-\delta}$  ( $x=0.5$ ). This data was collected at room temperature and under ambient pressure. The observed intensity is shown in blue, the calculated intensity is shown in red, and the difference is shown in grey underneath. Vertical markers indicate Bragg reflections of 96.95(1) wt.% P5S5FO (top) and 3.05(1) wt.%  $\text{Pr}_2\text{FeO}_4$  (bottom) phases ( $R_{\text{wp}} = 5.24\%$ ,  $R_{\text{Bragg}} = 1.32\%$ ).

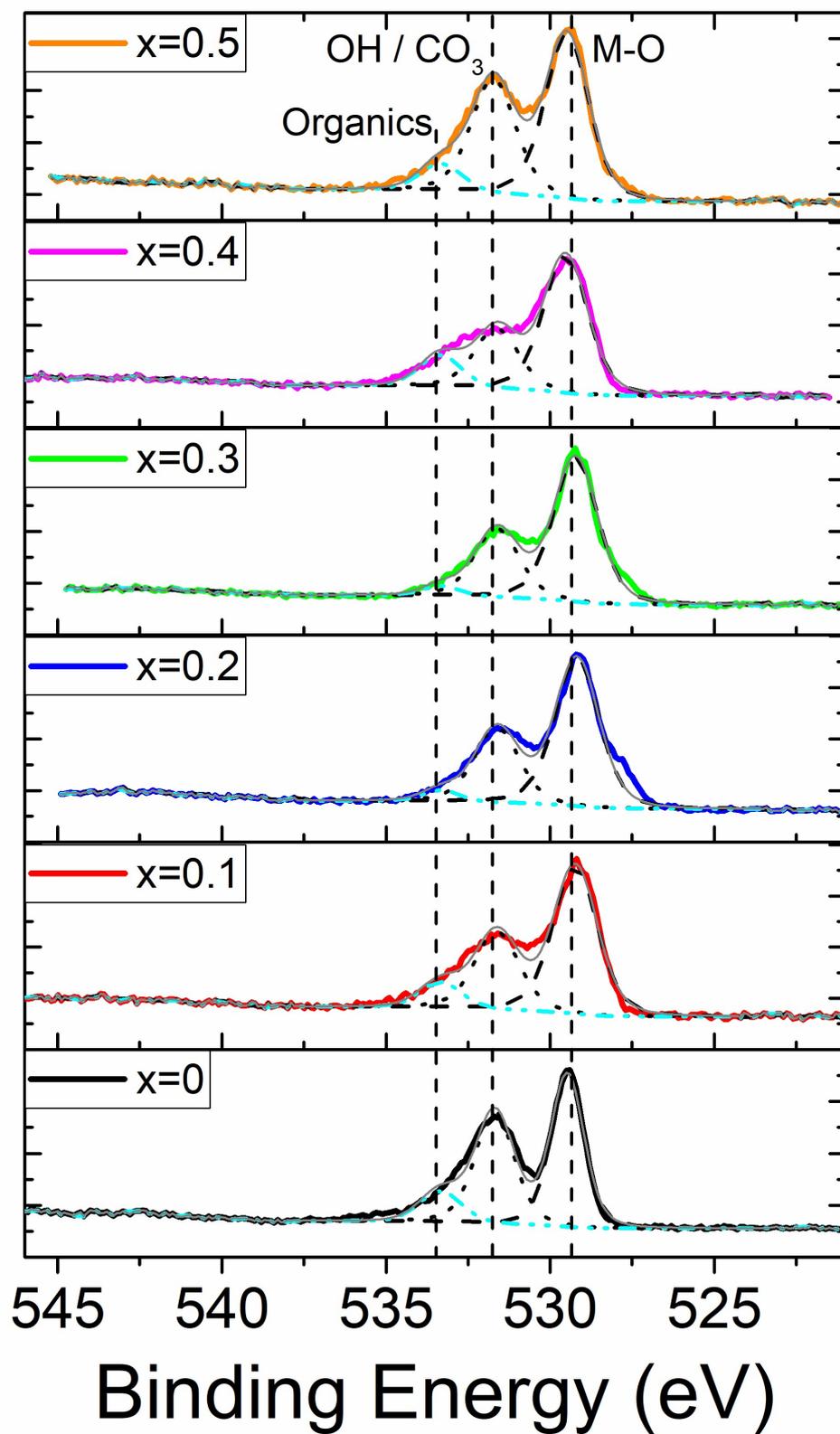


Figure S7 – Deconvoluted X-Ray Photoelectron Spectroscopy (XPS) scans of the O 1s core orbitals for the PSFO perovskite oxide catalyst series where dashed, dotted and cyan dashed lines show contributions from M-O lattice oxygen, OH / CO<sub>3</sub>, and organics, respectively. Grey lines indicate peak fitting, with all samples showing good fit.

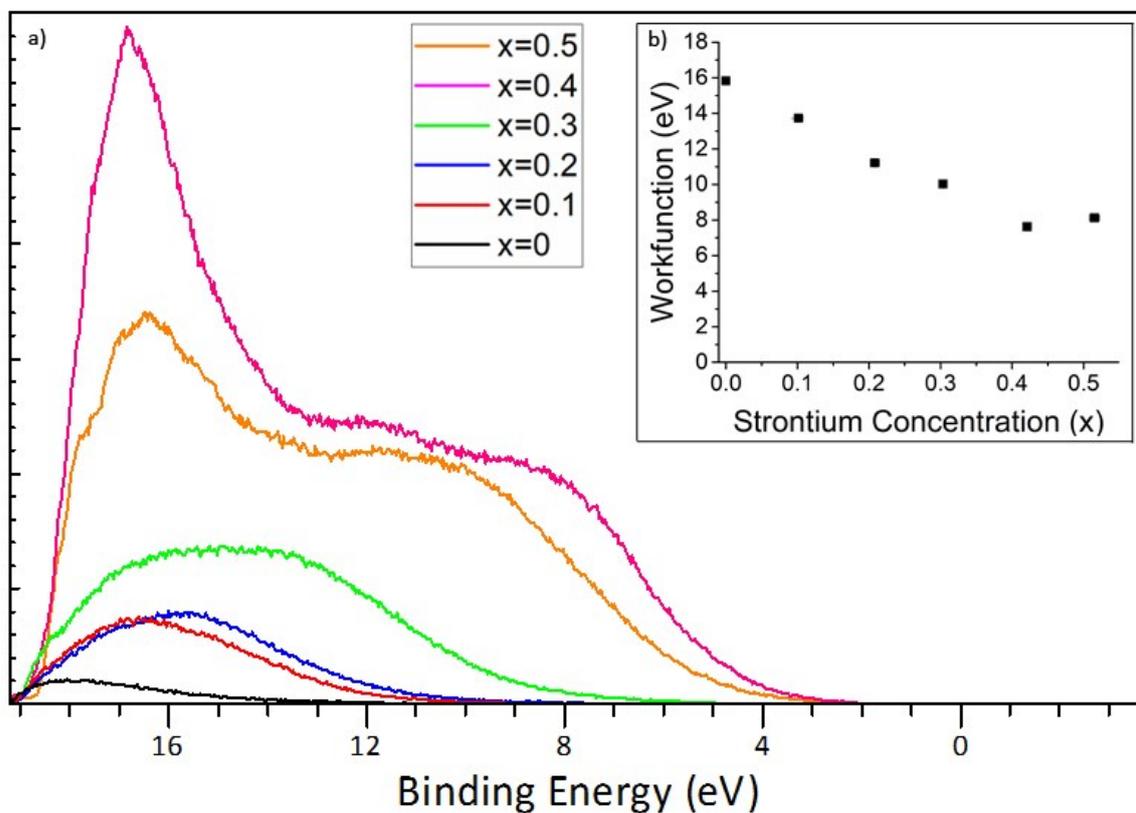


Figure S8 – a) Ultraviolet photoelectron spectroscopy (UPS) of PSFO perovskite catalysts. UPS Scans were used to calculate the workfunction values. b) Workfunction as a function of Sr<sup>2+</sup> concentration.

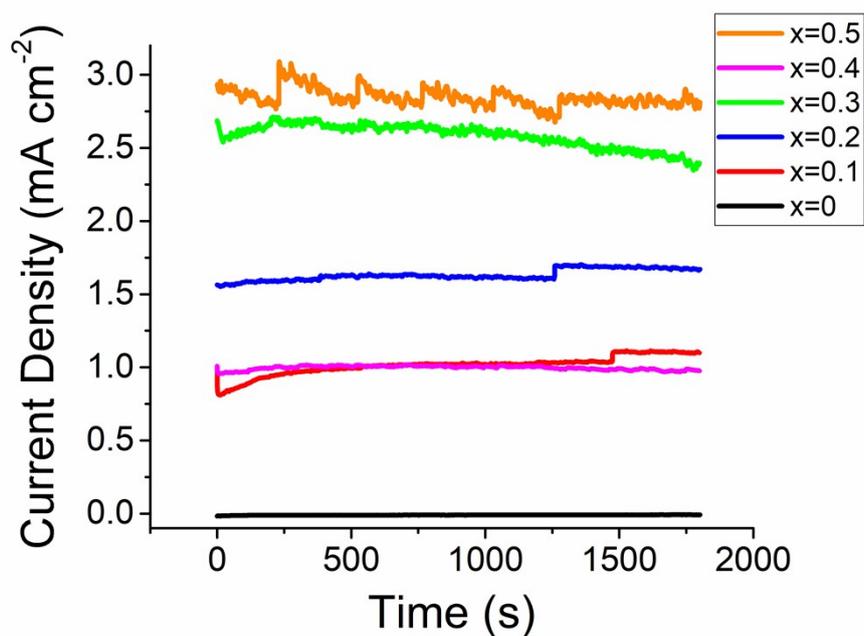


Figure S9 – Chronoamperometry measurements taken at 1.70 V<sub>RHE</sub> for 30 minutes in 0.1 M KOH electrolyte.