Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

A Single-/Double-Perovskite Composite with Overwhelming Single-Perovskite Phase for Oxygen Reduction Reaction at Intermediate Temperatures

Part I. Supplementary Data

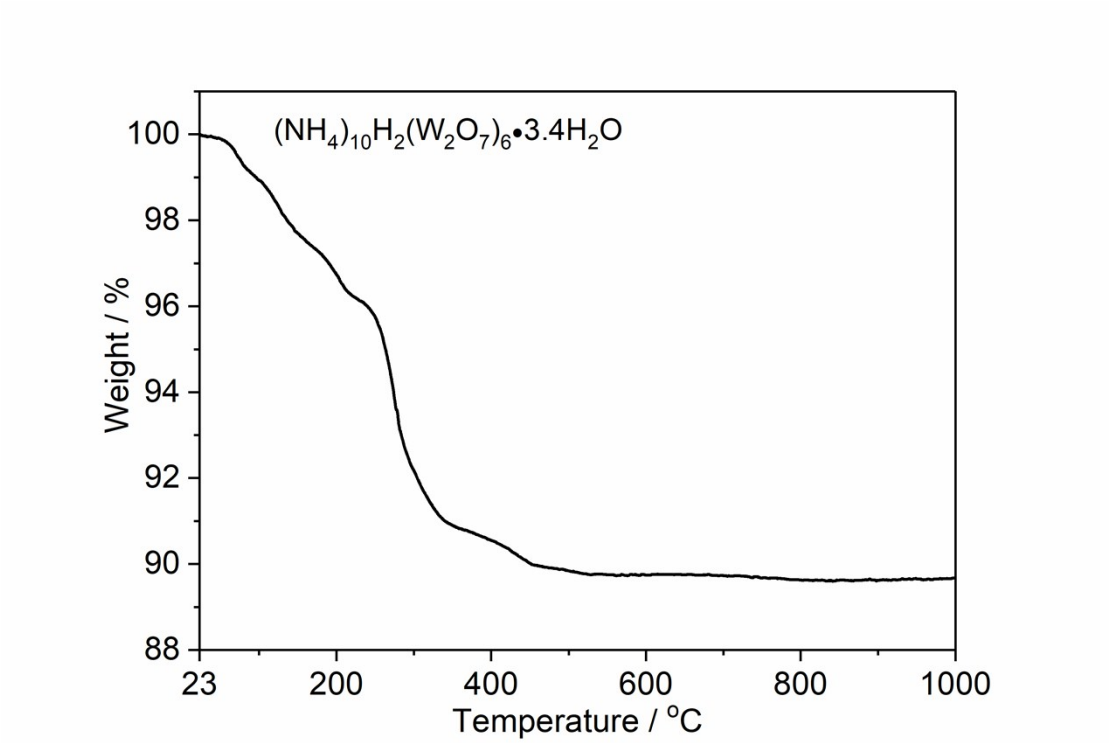

Figure S1. TG analysis of $(NH_4)_{10}H_2(W_2O_7)_6 \cdot xH_2O$ in Air. As temperature increased, the ammonium tungstate will decompose and form thermal stable WO3 product. Then, the number of crystal water in raw ammonium tungstate is calculated based on mass loss during thermal treatment.

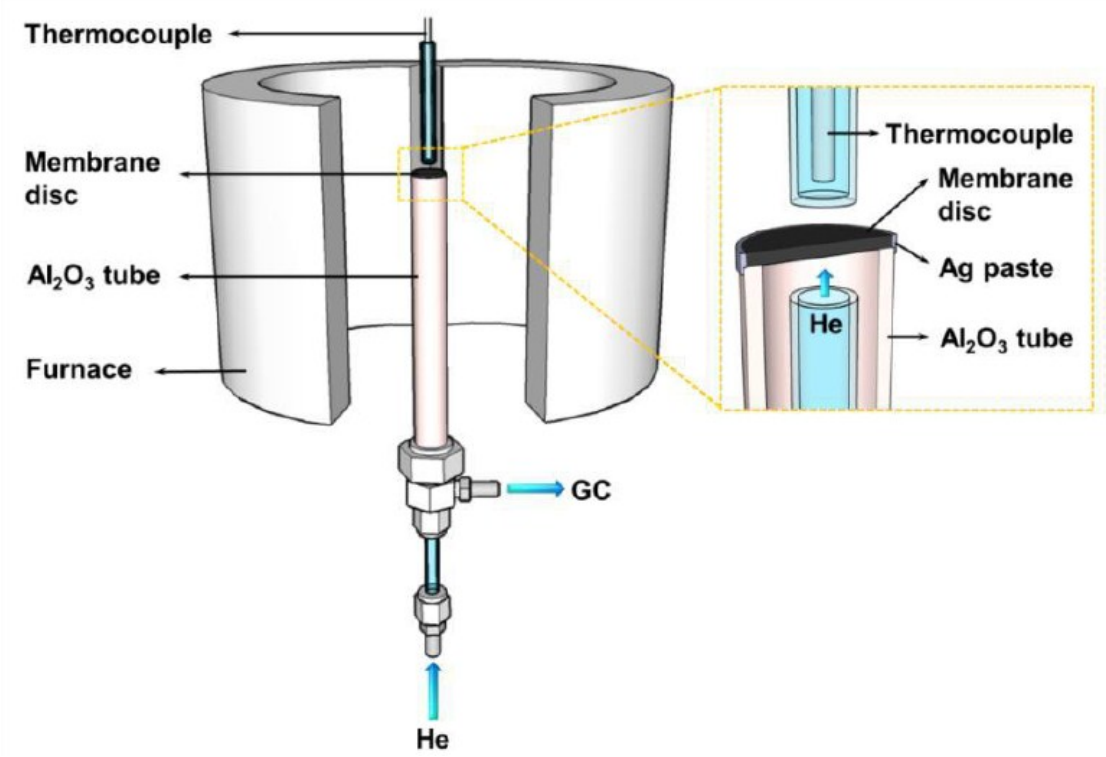

Figure S2. Home-constructed high-temperature oxygen permeation device.

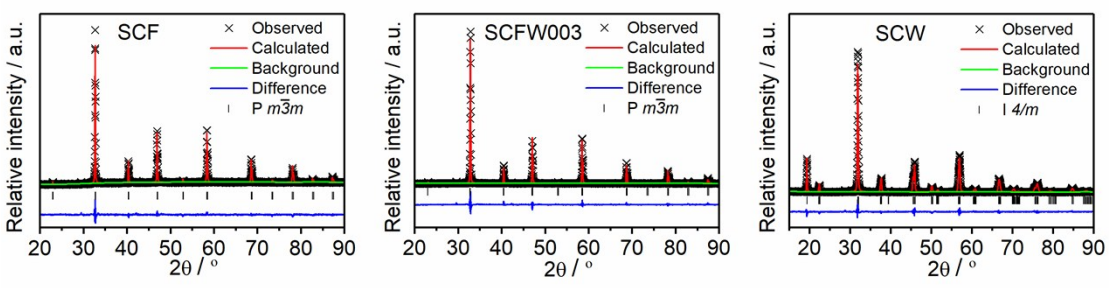

Figure S3. Refined XRD patterns of as prepared SCF, SCFW003 and SCW samples. The lattice parameters for SCF are a=b=c=3.8675(2); The lattice parameters for SCFW003 are a=b=c=3.86310(3); The lattice parameters for SCW are a=b=5.5875(1), c=7.9613(2); The reliability factors for the SCF are R_{wp}=4.37%, R_p=3.34%, x^2=1.709; The reliability factors for the SCFW003 are R_{wp}=3.97%, R_p=2.81%, x^2=3.132; The reliability factors for the SCW are R_{wp}=6.40%, R_p=5.07%, X^2=1.920.

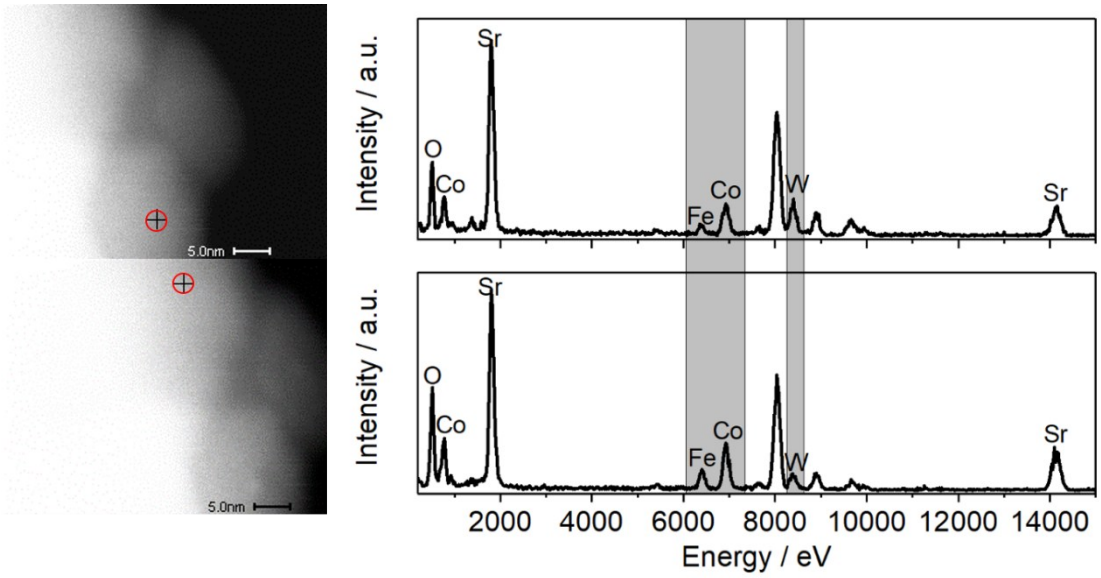

Figure S4. STEM-EDS point analysis of a as prepared SCFW sample.

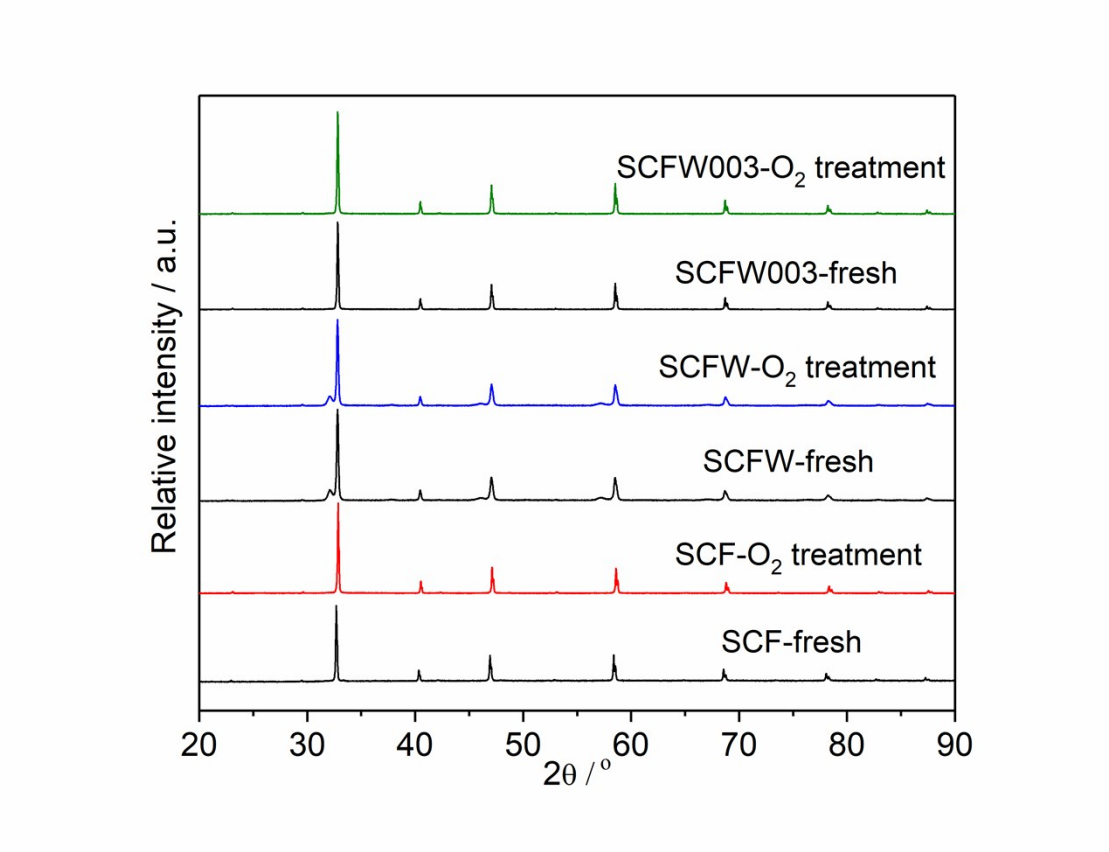

Figure S5. XRD patterns of SCF, SCFW and SCFW003 samples after 2h thermal treatment at 600 ^{o}C in O_2 atmosphere.

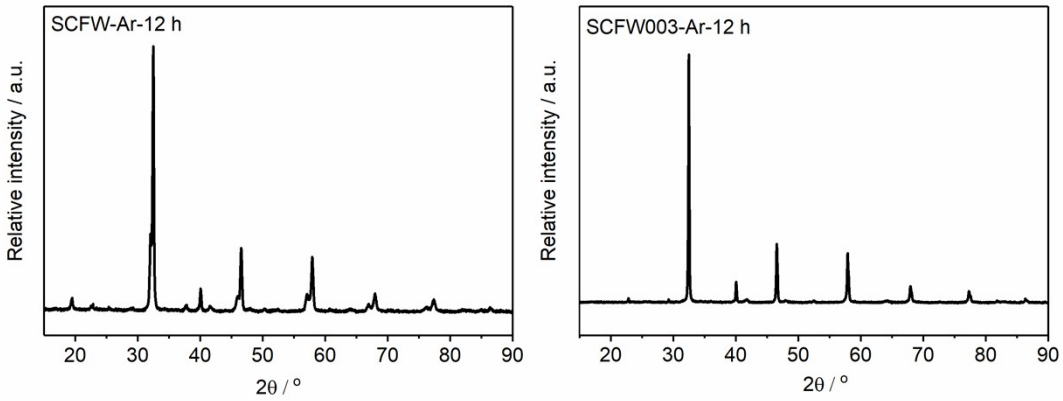

Figure S6. XRD patterns of SCFW and SCFW003 samples after 12h thermal treatment at 600 ^{o}C in Ar atmosphere.

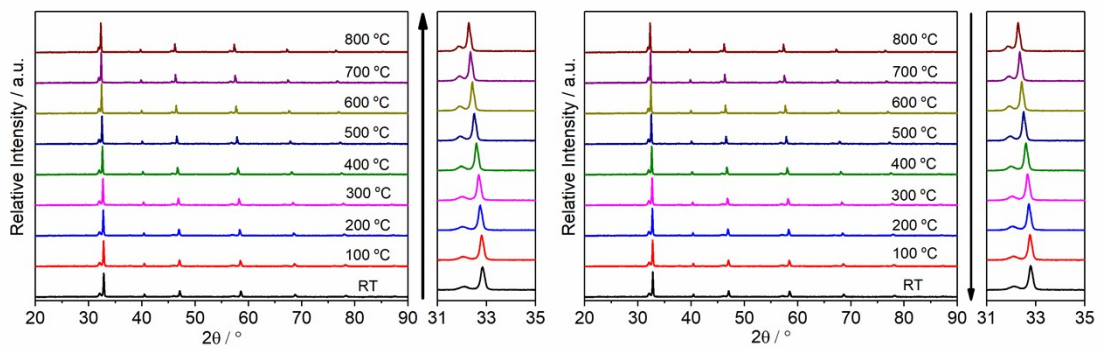

Figure S7. XRD patterns of the SCFW sample at various temperatures during the heating process and the cooling process. At each test temperature point, 5 min was allowed for the phase stabilization. No phase transition was observed during both the heating and cooling processes between room temperature and 800 °C. A shift of the diffraction peaks to the lower angle from heating process or to the higher angle during cooling process was observed, which was related to the thermal and/or chemical expansion/contraction of the oxide lattice.

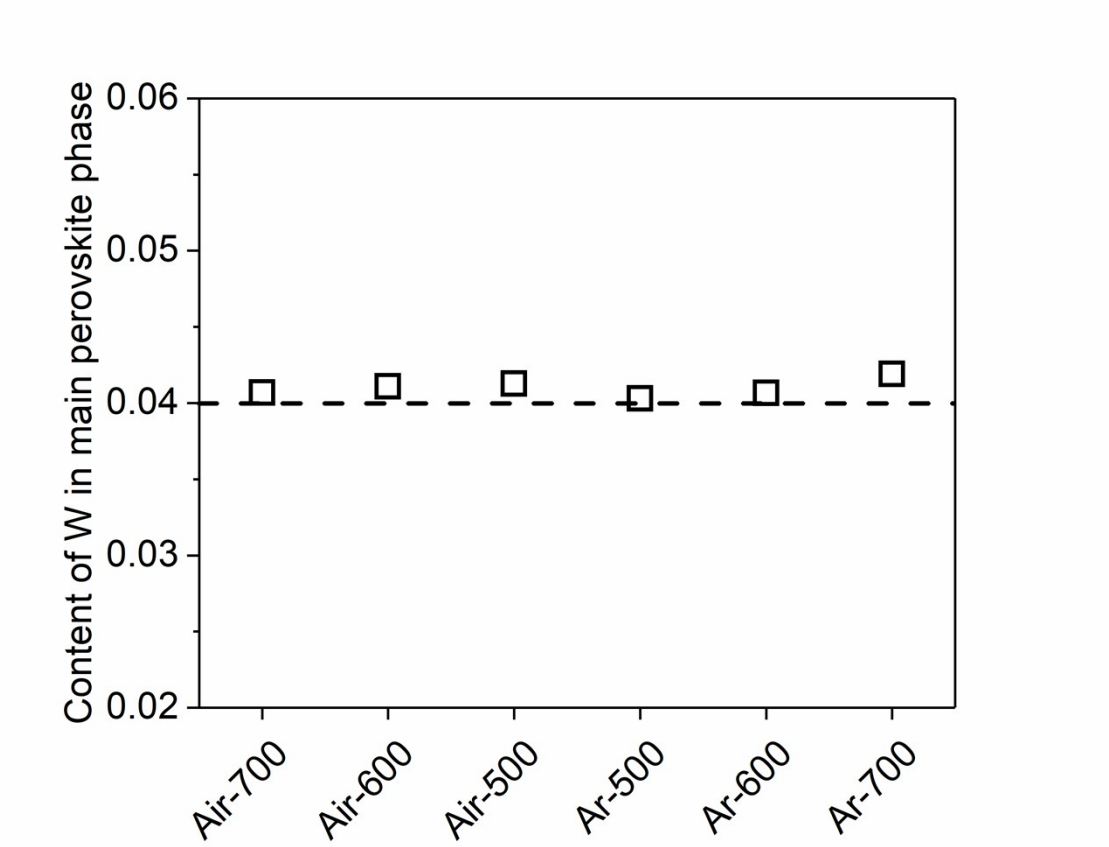

Figure S8. The possible W content in the SP phase for the various quenched SCFW samples.

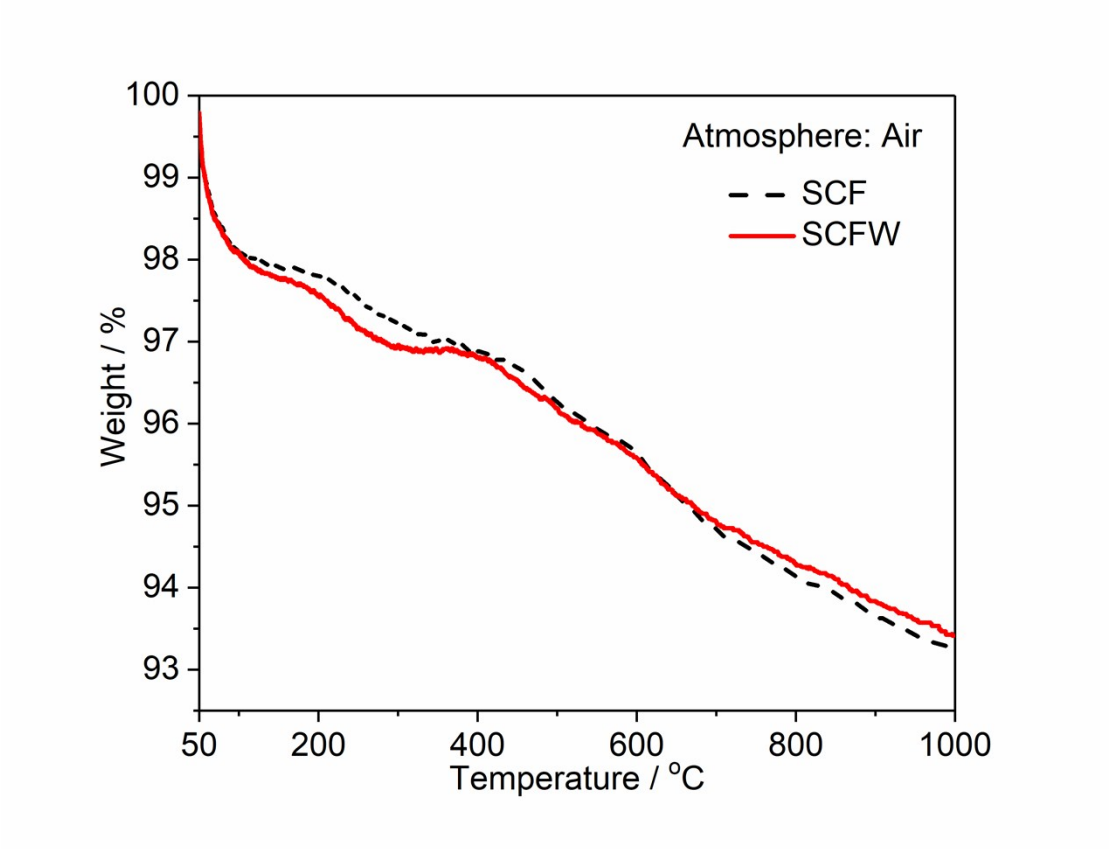

Figure S9. TG-MS analysis of SCF and SCFW in Air.

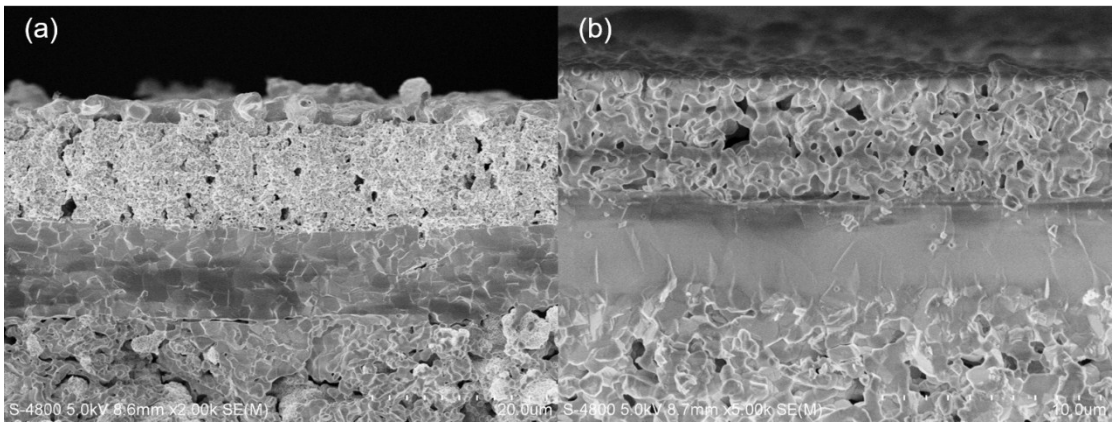

Figure S10. SEM of cross-sections of two single cells with either SDC (a) or YSZ (b) as the electrolyte.

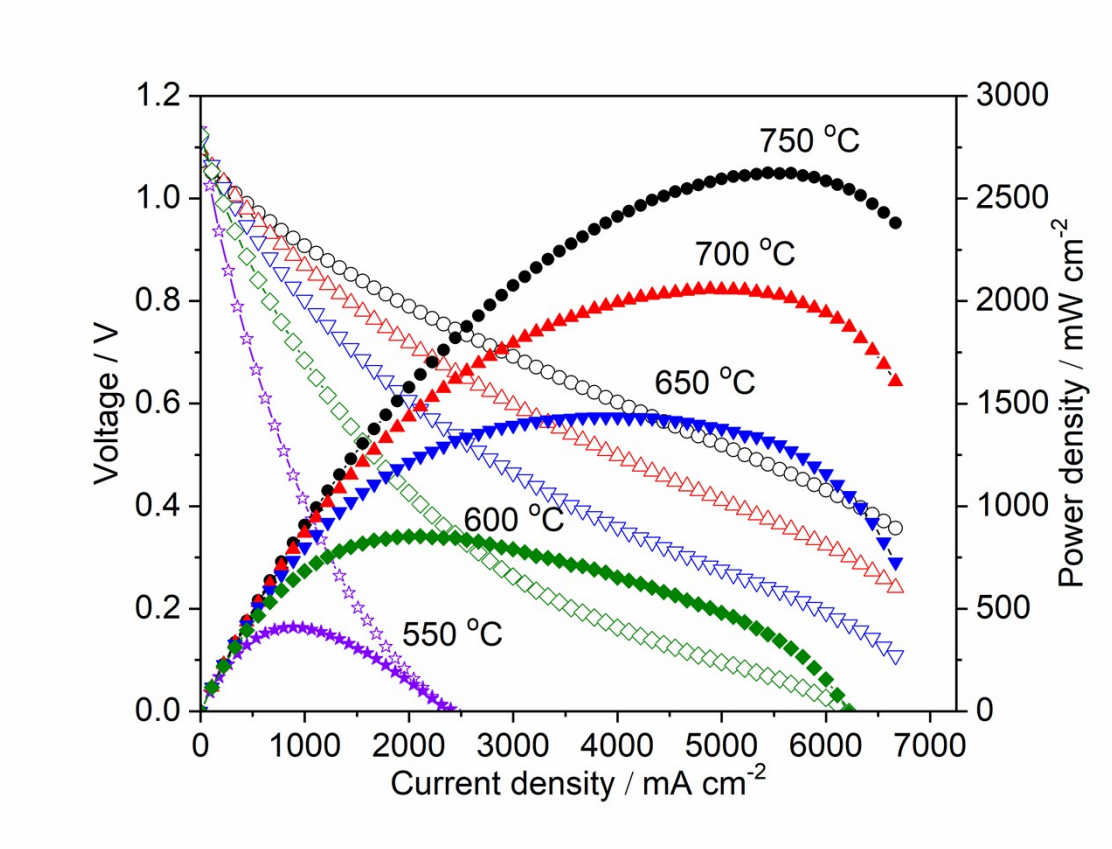

Figure S11. *I-V* and *I-P* curves of a Ni+YSZ supported single cell with SCFW cathode operating on hydrogen.

Part II Supplementary Note for Rietveld Refinement of SCFW

The Rietveld refinement is performed with a GSAS-EXPGUI package. The vibrational parameters (Uiso) for cations occupying the same site in the SP phase were constrained to be equal. During the refinement, we assume the B-site of SP is fully occupied by Co and Fe with a mole ratio of 9:1. This assumption is reasonable: 1) the real content of W in SP is very low and final results do not change a lot if assuming 4% W occupies the B-site in SP; 2) The atomic scattering factors for Co and Fe are close to each other. For DP phase, a standard Sr_2CoWO_6 (ICSD 190593) is used as the initial model. Due to the relative weak intensity diffraction peaks from DP, the Uiso values are not refined with a default value of 0.025 and fractional coordinates of O are also not refined. Moreover, since good fitting results can be obtained, the W and (Co, Fe) in DP phase are assumed totally disordered. Similar to the case in SP phases, 10% Co is replaced by Fe. The real content of W in the B-site of SP is determined from the refined mass ratio of SP phase. We caution that relative large error may exist between real mass ratio of SP phase and the values obtained from XRD refinement. However, the W content in SP phase is rather insensitive to the mass change. For example, if the mass ration of SP phase in SCFW varied between 80 wt.% and 90 wt.%, the W content in the B-site of SP will change between 3.82% and 4.49%. Thus, it is reasonable to estimate ~4% of the B-site is the SP phase is occupied by W based on a refined mass ratio of approximately 85 wt. % for the SP phase.