Fast redox kinetics in SrCo1-xSbxO3-δ perovskites for thermochemical energy storage and oxygen separation

George E. Wilson1, Ieuan D. Seymour1, Andrea Cavallaro1 Stephen J. Skinner\*1, Ainara Aguadero1\*

1Department of Materials, Imperial College London, Exhibition Road, London, SW7 2AZ, UK

**\* Correspondence:**Stephen Skinner  
s.skinner@imperial.ac.uk

Supplementary Material

Supplementary Table 1. Further DFT results comparing the undoped and 3.125% doped tetragonal structures.

|  |  |  |
| --- | --- | --- |
|  | **SrCoO3** | **SrCo0.96875Sb0.03125O3** |
| Possible Decomposition Products | SrCo6O11  Sr6Co5O15  O2 | SrCo6O11  Sr2Sb2O7  Sr6Co5O15  O2 |
| Fermi Energy  (eV) | 2.79 | 2.82 |

A picture containing text, black, white, crowd

Description automatically generated

Supplementary Figure 1. Scanning electron microscopy secondary electron images for Sb = 0.05 powder.

Chart, line chart

Description automatically generated

Supplementary Figure 2. Derivative of oxygen stoichiometry with respect to temperature for each of the Sb powders tested.

Chart, line chart

Description automatically generated

Supplementary Figure 3. Density of states plots for a) undoped and b) 3.125% doped   
SrCoO3-d structures.

|  |
| --- |
| a)  Chart  Description automatically generated |
| b)  Chart, histogram  Description automatically generated |
| c)  Chart, line chart, histogram  Description automatically generated |
| d)  Chart, histogram  Description automatically generated |

Supplementary Figure 4. Isothermal cycling data for SrCo0.95Sb0.05O3-δ at a) 500 °C, b) 600 °C, c) 700 °C and d) 800 °C.

|  |
| --- |
| a)  Chart, line chart  Description automatically generated |
| b)  Chart, line chart, histogram  Description automatically generated |
| c)  Chart, line chart, histogram  Description automatically generated |

Supplementary Figure 5. Isothermal cycling data for SrCo0.9Sb0.1O3-δ at a) 500 °C, b) 700 °C and c) 800 °C.

|  |
| --- |
| a)  Chart  Description automatically generated |
| b)  Chart  Description automatically generated |
| c)  Chart, line chart, histogram  Description automatically generated |
| d)  Chart, line chart, histogram  Description automatically generated |

Supplementary Figure 6. Isothermal cycling data for SrCo0.80Sb0.20O3-δ at a) 500 °C, b) 600 °C, c) 700 °C and d) 800 °C.

Graphical user interface, chart

Description automatically generated with medium confidence

Supplementary Figure 7. Comparison between XRD patterns of 5% Sb compound after 3 redox cycles.

A picture containing diagram

Description automatically generated

Supplementary Figure 8. Comparison between XRD patterns of 10% Sb compound after 3 redox cycles.

Chart

Description automatically generated

Supplementary Figure 9. Comparison between XRD patterns of 20% Sb compound after 3 redox cycles.