

“Tailoring Chemical Expansion by Controlling Charge Localization: *In Situ* X-ray Diffraction and Dilatometric Study of (La,Sr)(Ga,Ni)O<sub>3-δ</sub> Perovskite” by Nicola H. Perry, Sean R. Bishop, and Harry L. Tuller

### Supplementary Material

Table S-1. Change in Oxygen Stoichiometry vs. Oxygen Partial Pressure at 700 °C for La<sub>0.9</sub>Sr<sub>0.1</sub>Ga<sub>0.5</sub>Ni<sub>0.5</sub>O<sub>3-δ</sub>.

δ

| Log (pO <sub>2</sub> , atm) | Δδ      |
|-----------------------------|---------|
| -2.505                      | 0.00887 |
| -2.141                      | 0.00808 |
| -1.852                      | 0.00669 |
| -1.359                      | 0.00382 |
| -1.002                      | 0.00162 |
| -0.669                      | 0       |

Table S-2. Expansion vs. Oxygen Partial Pressure at 700 °C for La<sub>0.9</sub>Sr<sub>0.1</sub>Ga<sub>0.5</sub>Ni<sub>0.5</sub>O<sub>3-δ</sub>

| Log(pO <sub>2</sub> , atm) | ε <sub>C</sub> |
|----------------------------|----------------|
| -0.658                     | 0.00233        |
| -1.001                     | 0.00242        |
| -1.245                     | 0.00241        |
| -1.821                     | 0.00253        |
| -1.997                     | 0.00260        |
| -2.152                     | 0.00264        |
| -2.004                     | 0.00258        |
| -1.572                     | 0.00251        |
| -1.249                     | 0.00245        |
| -0.999                     | 0.00239        |
| -0.658                     | 0.00236        |

Table S-3. Change in Oxygen Stoichiometry vs. Oxygen Partial Pressure at 900 °C for La<sub>0.9</sub>Sr<sub>0.1</sub>Ga<sub>0.95</sub>Ni<sub>0.05</sub>O<sub>3-δ</sub>

| Log(pO <sub>2</sub> , atm) | Δδ       |
|----------------------------|----------|
| -0.675                     | 0.000217 |
| -1.048                     | 0.00232  |
| -1.456                     | 0.00404  |
| -1.902                     | 0.00593  |
| -2.193                     | 0.00716  |
| -2.564                     | 0.00881  |
| -2.202                     | 0.00672  |
| -1.909                     | 0.00604  |
| -1.458                     | 0.00430  |

Table S-4. Expansion vs. Oxygen Partial Pressure at 900 °C for La<sub>0.9</sub>Sr<sub>0.1</sub>Ga<sub>0.95</sub>Ni<sub>0.05</sub>O<sub>3-δ</sub>

| Log(pO <sub>2</sub> , atm) | ε <sub>C</sub> |
|----------------------------|----------------|
| -0.678                     | 0              |
| -0.987                     | 0.0000563      |
| -1.282                     | 0.000101       |
| -1.578                     | 0.000138       |
| -2.283                     | 0.000253       |
| -2.589                     | 0.000219       |
| -3.000                     | 0.000298       |

Table S-5. Change in Oxygen Stoichiometry vs. Oxygen Partial Pressure at 900 °C for La<sub>0.9</sub>Sr<sub>0.1</sub>Ga<sub>0.5</sub>Ni<sub>0.5</sub>O<sub>3-δ</sub>.

δ

| Log(pO <sub>2</sub> , atm) | Δδ        |
|----------------------------|-----------|
| -0.676                     | 0.0000102 |
| -1.024                     | 0.00696   |
| -1.387                     | 0.0149    |
| -1.878                     | 0.0263    |
| -2.160                     | 0.0330    |
| -2.525                     | 0.0414    |
| -2.165                     | 0.0331    |
| -1.881                     | 0.0267    |
| -1.391                     | 0.0158    |
| -1.030                     | 0.00802   |
| -0.687                     | 0.000831  |

Table S-6. Expansion vs. Oxygen Partial Pressure at 900 °C for La<sub>0.9</sub>Sr<sub>0.1</sub>Ga<sub>0.5</sub>Ni<sub>0.5</sub>O<sub>3-δ</sub>

| Log(pO <sub>2</sub> , atm) | ε <sub>C</sub> |
|----------------------------|----------------|
| -0.658                     | 0.00451        |
| -1.002                     | 0.00477        |
| -1.262                     | 0.00495        |
| -1.955                     | 0.00557        |
| -2.257                     | 0.00586        |
| -2.652                     | 0.00627        |
| -2.255                     | 0.00584        |
| -1.955                     | 0.00554        |
| -1.261                     | 0.00485        |
| -1.003                     | 0.00462        |
| -0.665                     | 0.00435        |