catalysts

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Supporting Info

High Temperature Water Gas Shift Reactivity of Novel Perovskite Catalysts

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1. Thermodynamic and Equilibrium Calculation for water gas shift (WGS)

For calculation of the curves in Figure S1, the following Equation (1) was used:

$$K_P = \frac{p_{CO_2} * p_{H_2}}{p_{CO} * p_{H_2O}} = \exp\left(\frac{4577,8}{T} - 4,33\right) \quad (1)$$

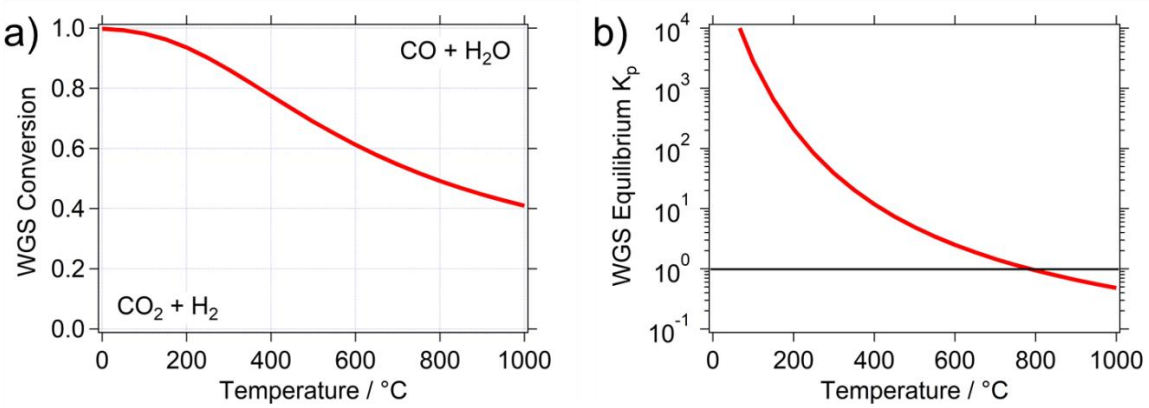

Figure S1: a) Thermodynamic limitation of the water gas shift (WGS) reaction. The higher the reaction temperature, the more pronounced the back reaction via reverse WGS is getting; b) reaction equilibrium plotted on a logarithmic scale plotted in dependence of the reaction temperature. At 800 °C K_P reaches the value of 1 where a 1:1 ratio of WGS educts and products is expected.

2. SEM prior to Catalytic Reaction

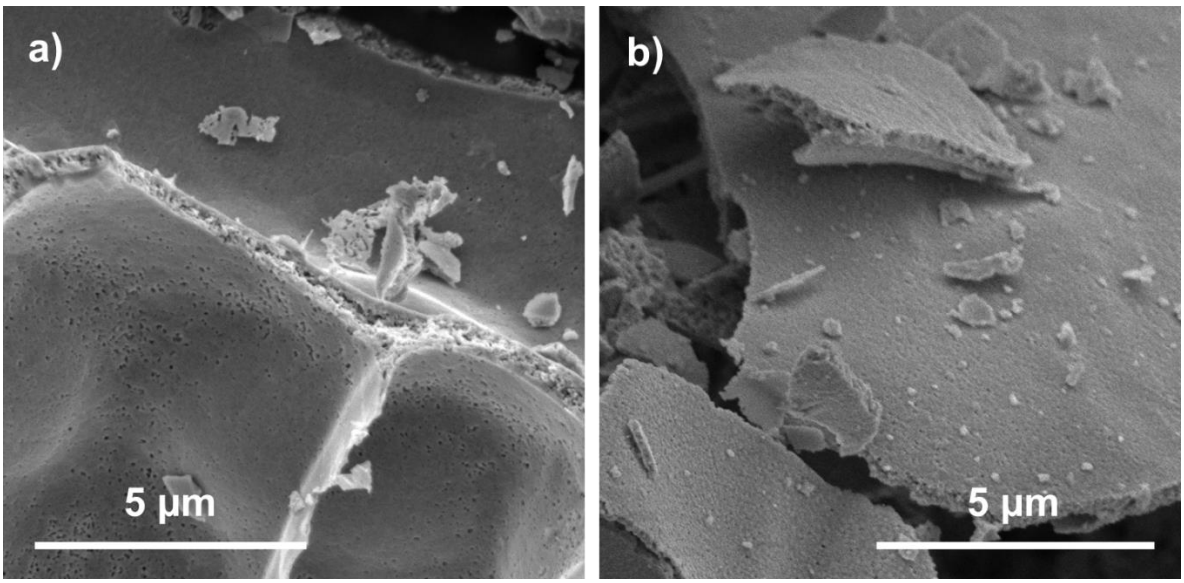

Figure S2: SEM Images of a) $Nd_{0.6}Ca_{0.4}Fe_{0.9}Co_{0.1}O_{3-\delta}$ and b) $Nd_{0.9}Ca_{0.1}FeO_{3-\delta}$ prior to catalytic reaction. The flakes on the surface are small pieces from the grinding after synthesis. No nanoparticles are observed before the catalytic reaction for the Co-doped perovskite.

3. Stability Tests for WGS Reactivity

To obtain the first insights into the long-term reaction stability of the novel perovskites, isothermal reactions were performed at 600 °C. We have chosen this high temperature to investigate the stability of the material under these harsh conditions and see if any rapid deactivation occurs. Below the results for the respective perovskites are shown (Figures S3-S7).

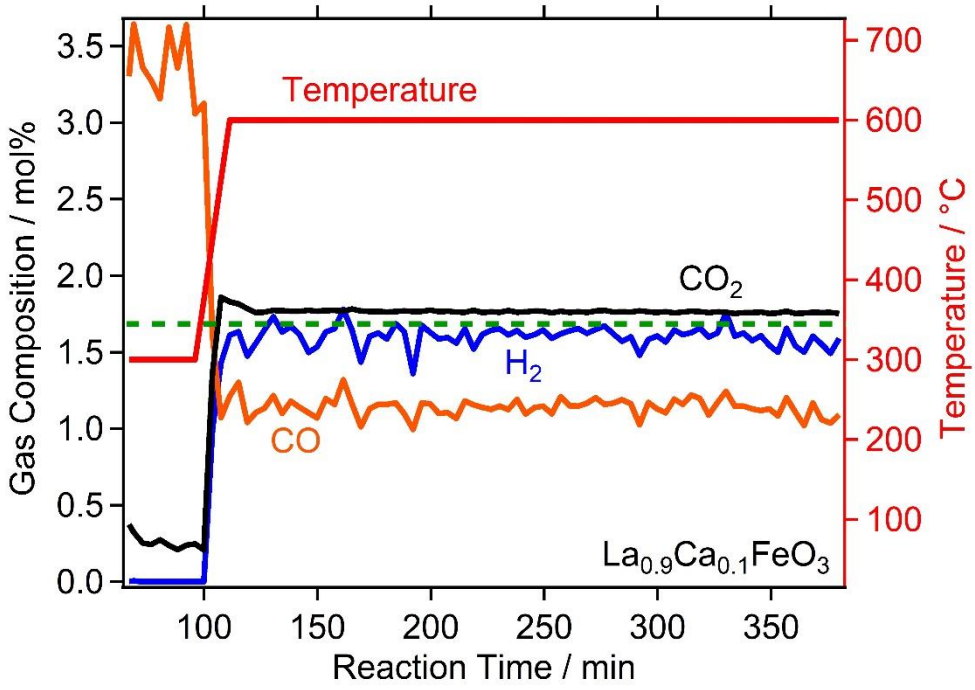

Figure S3: Isothermal WGS reaction at 600 °C for $La_{0.9}Ca_{0.1}FeO_{3-\delta}$. The dashed line serves as a guide for the eye. During the duration of the reaction (about 5 h), the catalyst showed stable reactivity without deactivation.

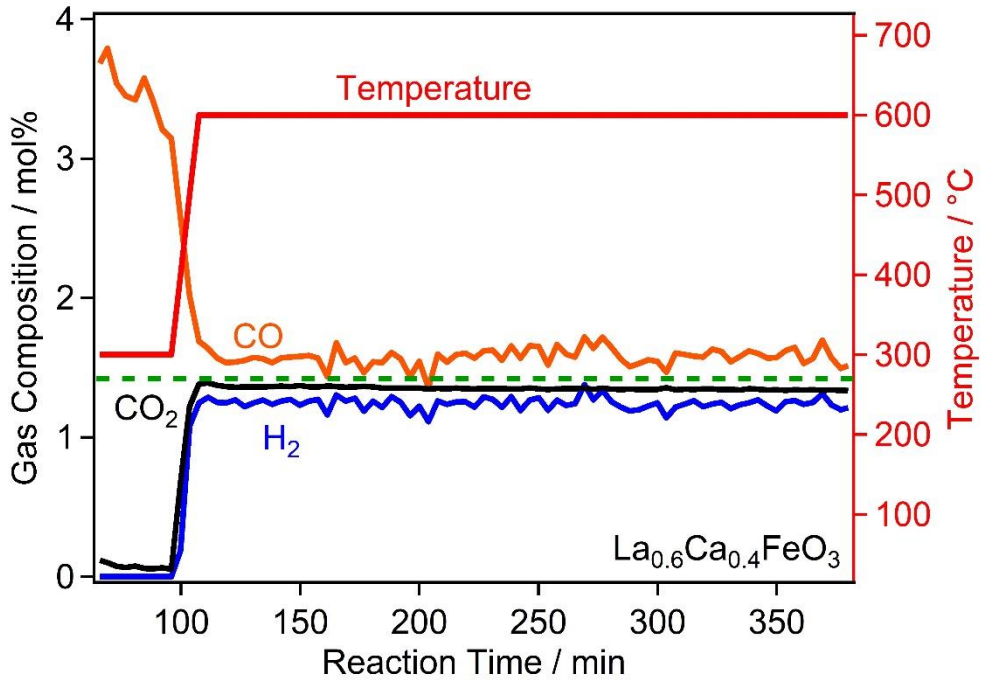

Figure S4: Isothermal WGS reaction at 600 °C for $La_{0.6}Ca_{0.4}FeO_{3-\delta}$. The dashed line serves as a guide for the eye. During the duration of the reaction (about 5 h) the catalyst showed stable reactivity without deactivation.

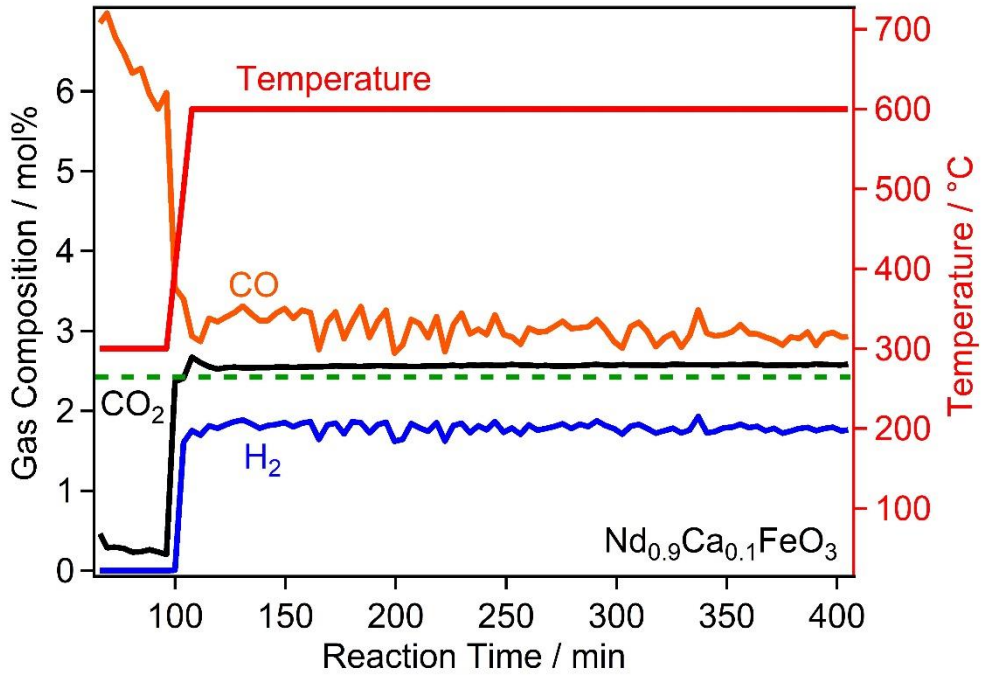

Figure S5: Isothermal WGS reaction at 600 °C for $Nd_{0.9}Ca_{0.1}FeO_{3-\delta}$. The dashed line serves as a guide for the eye. During the duration of the reaction (about 5 h), the catalyst showed stable reactivity without deactivation.

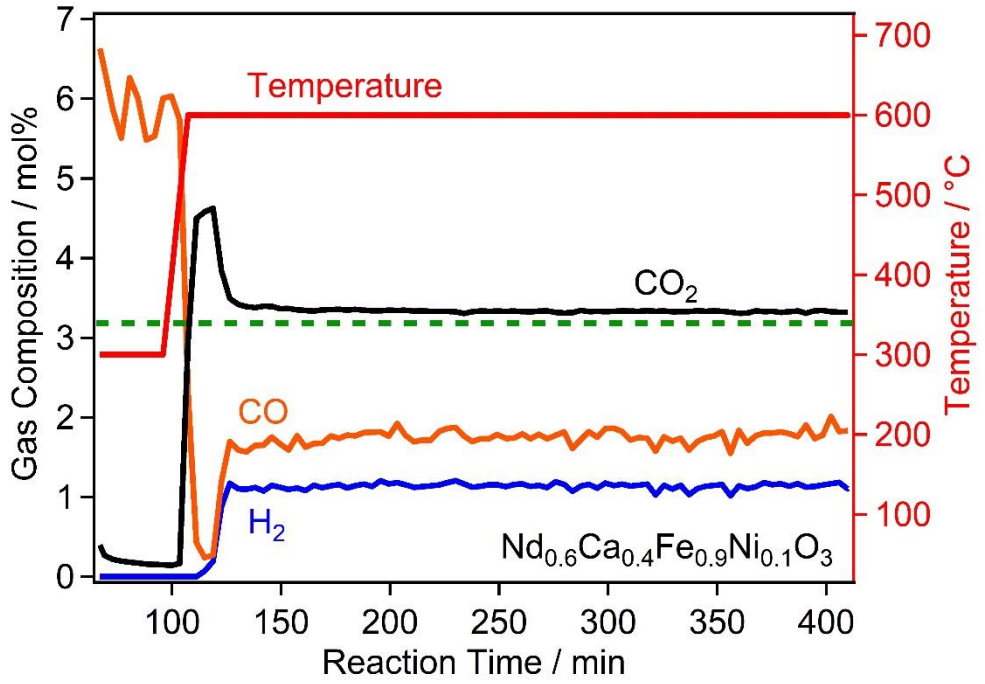

Figure S4: Isothermal WGS reaction at 600 °C for $Nd_{0.6}Ca_{0.4}Fe_{0.9}Ni_{0.1}O_{3-\delta}$. The dashed line serves as a guide for the eye. During the duration of the reaction (about 5 h) the catalyst showed stable reactivity without deactivation.

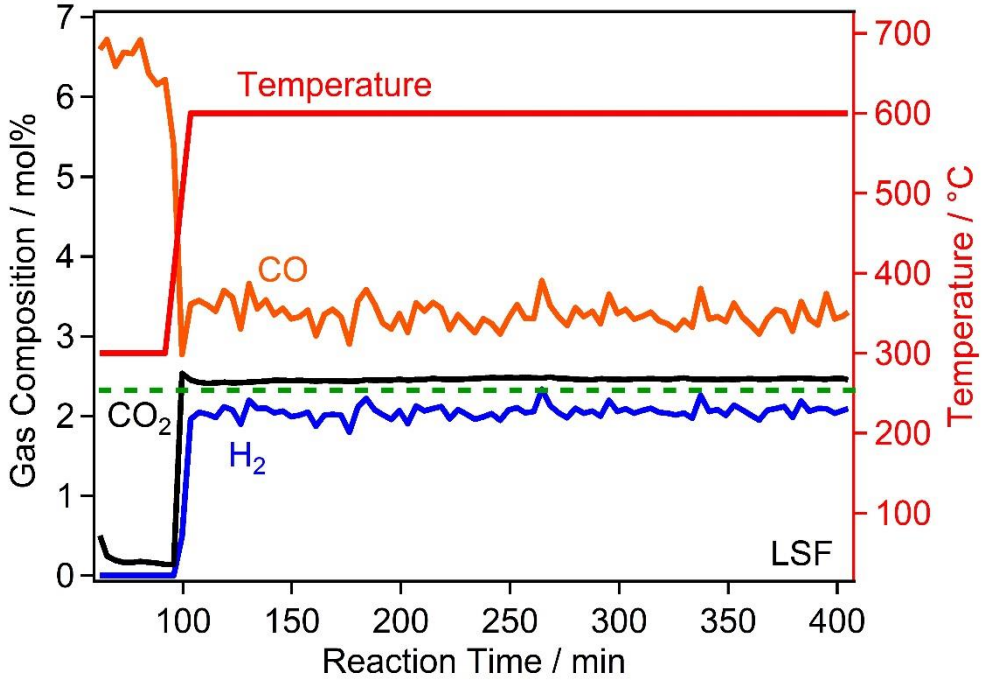

Figure S7: Isothermal WGS reaction at 600 °C for LSF. The dashed line serves as a guide for the eye. During the duration of the reaction (about 5 h), the catalyst showed stable reactivity without deactivation.

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Conflicts of Interest: The authors declare no conflict of interest.