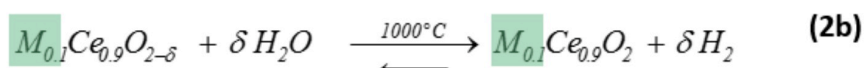
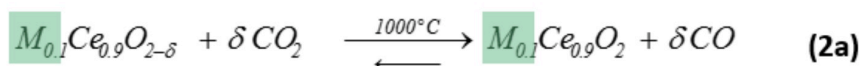
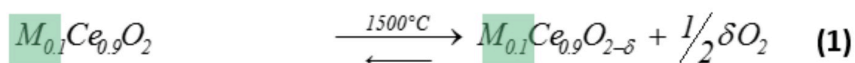


Dopant Screening of Ceria-Based Materials for Solar Thermochemical Two-Step CO₂-Splitting

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We consider the solar-driven 2-step thermochemical cycle for splitting H₂O and CO₂ via CeO₂-based redox reactions^[1]. In the first endothermic step, ceria is thermally reduced using concentrated solar energy by releasing O₂ (Eq. 1). In the second exothermic step (Eq. 2a and 2b), reduced ceria reacts with H₂O and/or CO₂ to generate H₂ and/or CO, respectively. The fuel yield is proportional to the oxygen exchange capacity (OEC), which can be improved with cationic doping.



Starting from our earlier work^[2] we investigate all possible tetravalent dopants of the periodic table because of their potential to yield higher OEC values due to flexible vacancy formation processes. The doped ceria samples were analyzed with a wide range of analytical techniques (e.g. PXRD, TG, ICP-MS, SEM-EDX, XAS). We found a correlation between the effective ionic radius and the OEC that was supported by DFT calculations. The tetravalent dopants with best redox performance were tested for their high temperature long-term stability in thermogravimetric cycling experiments.

[1] W.C. Chueh, C. Falter, M. Abbott, D. Scipio, P. Furler, S.M. Haile, A. Steinfeld, *Science* **2010**, 330, 1797.

[2] J.R. Scheffe, R. Jacot, G.R. Patzke, A. Steinfeld, *J. Phys. Chem. C* **2013**, 117, 24104.