

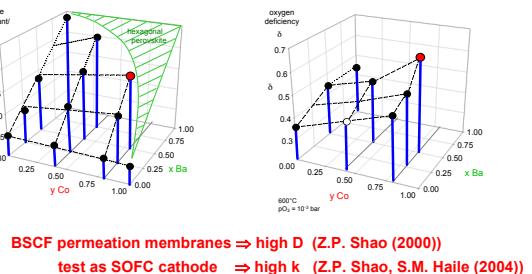
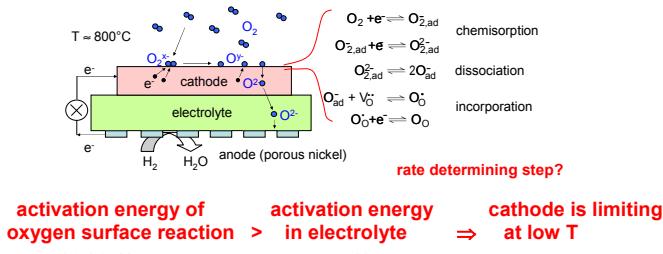


Oxygen exchange on $(\text{Ba}, \text{Sr})(\text{Co}, \text{Fe})\text{O}_{3-\delta}$

R. Merkle, L. Wang, J. Maier

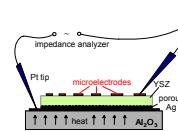
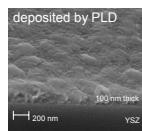
MPI for Solid
State Research
Stuttgart

$\text{Ba}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_{3-\delta}$ as SOFC cathode material:



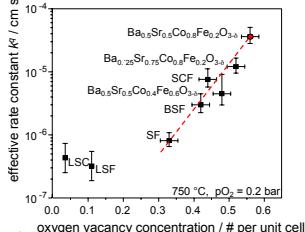
Experiments:

model system with well-defined morphology
 \Rightarrow intrinsic materials properties

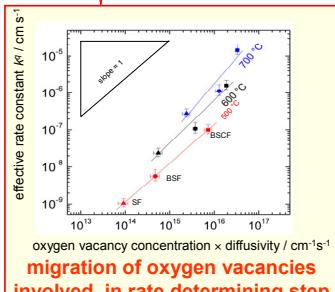
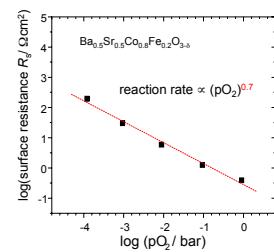
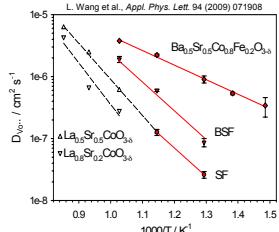


F.S. Baumann et al.,
Solid State Ionics 177 (2006) 1071

nonlinear correlation of k with $[V_O^-]$ in $(\text{Ba}, \text{Sr})(\text{Co}, \text{Fe})\text{O}_{3-\delta}$ materials:

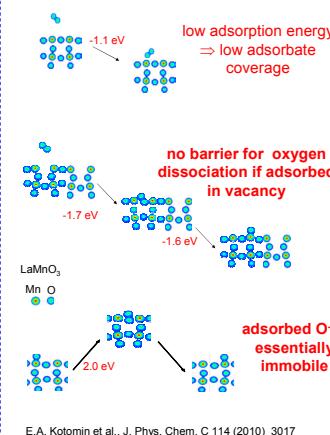


¹⁸O isotope exchange on BSCF films
L. Wang et al., Appl. Phys. Lett. 94 (2009) 071908

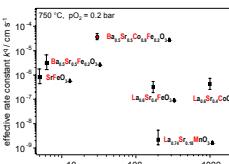


molecular oxygen species involved in rate determining step

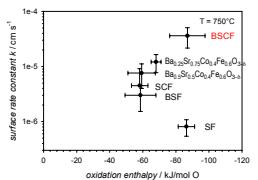
Theory: DFT calculations for $(\text{La}, \text{Sr})\text{MnO}_3$



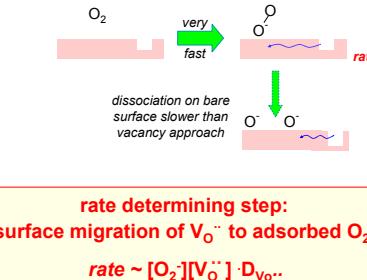
no correlation of rate constant with:



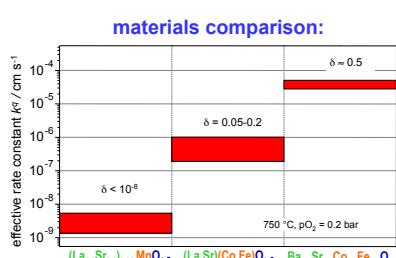
electronic conductivity in $(\text{Ba}, \text{La}, \text{Sr})(\text{Mn}, \text{Fe}, \text{Co})\text{O}_{3-\delta}$ perovskites



oxidation enthalpy in BSCF family



L. Wang, R. Merkle, J. Maier, J. Electrochem. Soc. 157 (2010) B1802



L. Wang, R. Merkle, J. Maier, ECS Transact. 257 (2009) 2497

Summary: - high V_O^- concentration and mobility decisive for fast surface exchange

\Rightarrow search for Ba-free cathode materials with high σ_{ion}

- DFT calculations for BSCF in progress

- defect model required to verify pO_2 -dependence and activation energy

- "in-situ XPS" for surface oxygen species, cation composition, ageing

Acknowledgement

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