

**Friday 8 November 2019**  
**16:00 Room: OFLG/402**  
**TFI-LMX SEMINAR**

## **Interaction of O<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O with Perovskite Surfaces. Insights from the Theory.**

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The interaction of small, energy-related gas molecules with materials' surfaces is at the frontier of materials science and molecular science and requires deep atomistic understanding of the materials' properties, surface reconstruction, heterogeneous catalysis, and molecules. Those processes are of fundamental importance for the performance and durability of energy devices, *i.e.*, fuel cells, electrolyzers, metal-air batteries, etc. The atomistic simulations are key for understanding the surface reactivity and gaining control over the desired chemical reaction. We apply first principle methods to understand the interaction of molecular oxygen with SrO and LaO terminated perovskites and Rurlsten-Popper series oxides. Our research provides understanding for the difference in catalytic activity of *alkaline-earth elements* versus *rare-earth elements* within the outermost perovskite layer. We have elucidated the reaction mechanism for oxygen reduction reaction for those surfaces and its relation to the surface oxide vacancy population. We have studied the formation of a surface SrCO<sub>3</sub> layer and various possible products of H<sub>2</sub>O interaction with the SrO surface, such as, surface chemisorbed water and the formation of a surface hydroxide layer [1-5]. The co-adsorption of CO<sub>2</sub> and H<sub>2</sub>O was explained both theoretically and experimentally showing that its products follow a complex temperature dependence and as a result, the surface composition may vary between carbonate and surface chemisorbed water. Our theoretical simulations have shown that the presence of water molecules in the gas phase might assist the molecular oxygen/lattice oxygen exchange reaction by stabilization of the surface oxo species in the transition state with a hydrogen bond mechanism. As a result, the activation barrier for molecular oxygen dissociation is decreased leading to an increase in the surface exchange rate constant. Our study demonstrates that the SrO terminated SrTiO<sub>3</sub> surface is not static but instead, dynamically responds to external factors such as gas composition, humidity, and temperature. As a result, the surface phases can show different trends for the surface exchange reaction with molecular oxygen by either an increase or decrease in the exchange rate.

### **References:**

- 1) A. Staykov, H. Tellez, J. Druce, J. Wu, T. Ishihara, J. Kilner, *Sci. Tech. Adv. Mater.* 19, 221 (2018).
- 2) A. Staykov, S. Fukumori, K. Yoshizawa, K. Sato, T. Ishihara, J. Kilner, *J. Mater. Chem. A* 6, 22662 (2018).
- 3) J. Wu, K. Fujii, M. Yashima, A. Staykov, T. Akbay, T. Ishihara, J. Kilner, *J. Mater. Chem. A* 6, 11819 (2018).
- 4) Franziska Hess, Aleksandar T Staykov, Bilge Yildiz, John Kilner, *Handbook of Materials Modeling: Applications: Current and Emerging Materials* 1-31 (2018).
- 5) A. Staykov, H. Tellez, T. Akbay, J. Druce, T. Ishihara, J. Kilner, *Chem. Mater.* 27, 8273-8281 (2015).

### **About the speaker**

Aleksandar Staykov obtained his PhD in 2006 from Wilhelm Ostwald Institute for Physical and Theoretical Chemistry, Leipzig University, Germany. He was a postdoctoral researcher at the Institute for Materials Chemistry and Engineering, Kyushu University, Japan from 2006-2010. In 2011 he joined the International Institute of Carbon-Neutral Energy Research, Kyushu University, Japan as an assistant professor. In 2016 he became associate professor and principle investigator. His laboratory is focusing on atomistic simulations of chemical processes at surfaces and interfaces.