

## Vortragsankündigung

**Mittwoch, 6. November 2019, 11.15 Uhr**

Seminarraum I (JAK2AOG1.33), Jakob-Haringer-Straße 2a

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## **“Probing the Active Surface of Metal Oxide Catalysts”**

The nature of the chemical bond in metal oxides ranges from purely ionic to essential covalent, which is reflected in diversified functional properties. In heterogeneous catalysis over metal oxides the delicate interplay between electronic bulk structure and surface termination is used to control the activation of molecules on the catalyst surface and to govern selectivity in complex reaction networks.<sup>1</sup>

In our work we investigate the reactive surface of metal oxide catalysts in activation of C-H, O-O, C-O, and O-H bonds in small molecules. The present talk describes our approach using two examples: (i) alkaline earth oxides in the oxidative coupling of methane to ethane and ethylene, and (ii) perovskites in the oxidation of propane.

Even though the bond dissociation energy of methane is large with 423 kJ/mol, the activation of oxygen is much more important to direct the selectivity towards the desired products in the oxidative coupling of methane over basic, non-reducible oxides, such as MgO or CaO. It will be shown that the capability of the material to activate oxygen is directly linked to the catalytic performance.<sup>2</sup>

In reducible transition metal oxide catalysts, the abundance of highly reactive electrophilic surface oxygen species is controlled by a self-limiting charge carrier transport situation that is created by surface modification under the influence of the gas phase resulting in band bending.<sup>1</sup> Due to their structural and chemical versatility, pure or partially substituted  $AA'A''BB'B''(O,X)_3$  perovskites have been selected as model system to investigate the universality of such a concept in oxidation catalysis. It is explored whether surface modifications can turn an unselective combustion catalyst into a selective catalyst in oxidation of propane in presence of gas-phase oxygen. Increased concentration of OH species, and higher abundance of adsorbed activated oxygen in presence of auxiliary steam in the feed account for a more selective situation.

[1] P. Kube, *et al.*, Functional Analysis of Catalysts for Lower Alkane Oxidation, *ChemCatChem* **2017**, 9, 573-585.

[2] L. Thum, *et al.*, Oxygen Activation in Oxidative Coupling of Methane on Calcium Oxide, *The Journal of Physical Chemistry C* **2019**, 123, 8018-8026.