

# UniCat Colloquium

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## *In situ TEM and X-ray spectroscopy studies of manganite perovskite electro-catalysts for water oxidation*

In-situ studies of catalysts are of high interest since they offer the opportunity to study their atomic and electronic structure in the active state. We present environmental Transmission Electron Microscopy (ETEM) and X-ray absorption spectroscopy (XAS) studies of O<sub>2</sub> evolution catalysis at conditions close to H<sub>2</sub>O splitting in various doped manganite perovskite and Ruddlesden-Popper phases. These systems offer the opportunity for fundamental studies of factors controlling the active site, surface structure and defect chemistry in water splitting and oxygen evolution.

In manganites, such as Pr<sub>1-x</sub>CaxMnO<sub>3</sub> ( $x > 0.3$ ), where the acceptor sites are strongly influenced by oxygen 2p bands, lattice oxygen is involved as an active site in water splitting and oxygen evolution. This has the consequence that surface oxygen vacancies are formed which can migrate into the subsurface and in turn initiate electrode corrosion. In contrast, our studies of manganites, where the hybridization to the oxygen 2p state is less pronounced, such as Pr<sub>1-x</sub>CaxMnO<sub>3</sub> ( $x < 0.2$ ) or La<sub>1-x</sub>SrxMnO<sub>3</sub> (0.4), activity scales with Mn surface concentration and Mn is oxidized during OER. Active states of such electrodes show a highly dynamic motion of Mn surface vacancies, being relevant for mechanistic understanding of the O-O bond formation process. The different behavior of the selected manganites with respect to defect chemistry under OER conditions is explained based on ab initio calculations, where the doping trends are correlated to induced changes of the electronic band structure.

The talk will include careful studies of beam-induced effects in in-situ ETEM and XAS studies, in order to give support the significance of the in situ observations for real world electro-chemistry.

**Wednesday, May 02, 2018 at 5:15 PM**

TU Berlin, Institute of Chemistry  
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

**Prof. Dr. Dau (FUB)**

Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!  
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - [www.unicat.tu-berlin.de](http://www.unicat.tu-berlin.de)



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