

EPFL Valais/Wallis SEMINAR

13. 3. 2020, 11:00 - 12:00, EPFL Valais/Wallis in Sion, 4th floor, Zeuzier Room

Hydride Surfaces for Catalysis

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Because of its relevance in catalysis, the interaction of hydrogen with metallic surfaces is generally well studied. However, knowledge on surface properties is limited when it comes to the class of metals, which form hydrides, such as titanium. Hydride surfaces have peculiar properties for their application as heterogeneous hydrogenation catalysts, e.g., they may have even less hydrogen on the surface than their metallic counterparts resulting in lower catalytic yields. I will discuss two archetypal hydrides: CO₂ methanation is catalyzed by various hydride-forming intermetallics because they supply highly reactive atomic hydrogen [1]. In contrast, on palladium surfaces the formation of the hydride PdH_x decreases the reaction rate for the Sabatier reaction [2].

Titanium dihydride TiH₂, though, has been recently shown to catalyze the ammonia synthesis under Haber-Bosch conditions while titanium metal shows no activity [3].

The key to understanding the catalytic properties of hydrides is their electronic structure. The standard electron spectroscopy methods are incompatible with hydrogen pressures needed to form hydrides, therefore these kind of experiments are usually restricted to post-mortem analysis. We have developed a method to hydrogenate thin films in-situ under UHV conditions compatible with electron spectroscopy measurements. The capabilities of this system are demonstrated on the example of Ti/TiH₂ and discussed in relation with the current understanding that hydrogen vacancies play a major role in the activity towards ammonia synthesis.

References:

- [1] Kato et al., *Angew. Chem. Int. Ed.*, **55** (2016), 6028
- [2] Billeter et al., *ChemPhysChem*, **20** (2019), 1398
- [3] Kobayashi et al., *J. Am. Chem. Soc.*, **139** (2017), 18420



Born in Solothurn, Switzerland in 1992, Emanuel Billeter graduated from ETH Zürich with a MSc in Chemistry in 2018. For his master thesis under the supervision of Prof. N. Stadie, he went to Montana State University to work on Phosphorus doped graphitic carbon. In 2018 he joined the Laboratory of Advanced Analytical Technologies at Empa for his PhD Project to work on high-pressure XPS of metal hydrides and their catalytic properties.