Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Institute for Molecular Physical Science (IMPS)

Einladung zu einem Kolloquium

Datum/Zeit:	**Dienstag, 19.11.2024, 16.45 Uhr**
Referent:	**Prof. Susanne Mossin** Technical University of Denmark, -DTU, Lyngby, Denmark
Titel:	In-situ and operando Electron Paramagnetic Resonance applied for investigation of copper zeolite based catalysts
Ort:	**HCI G7**

A key feature of the copper-based catalyst applied commercially to remove NO and NO_2 from the exhaust of combustion engines is the ability of copper to change oxidation state. The reaction is known as the Selective Catalytic Reduction (SCR). Fortunately, copper (II) gives an informative and quantifiable EPR signal even at the reaction conditions of the catalyst above 250 °C. This can be used to obtain information about the catalyst, which is impossible to obtain in any other way, such as the steady-state distribution of copper species in a working catalyst bed.
We have developed a methodology to investigate heterogeneous catalysts using CW EPR spectroscopy on the reactor configured for catalytic reactions. We have applied several types of protocols to extract useful information about the amount of reactive metal, the identity of the active metal species and the time-resolved reaction dynamics of the catalyst.
The influence of the chabazite (CHA) zeolite framework on the reactive copper centers will be illustrated.[1] This includes the topology of the zeolite as well as the total amount and the local distribution of aluminum in the structure, which depends upon the synthesis method of the zeolite.[2] The method of introduction of copper into the material is largely unimportant, however, due to the very high mobility of copper at reaction conditions.
Our recent results on catalyst deactivation by sulfur species [3] shows that the rate of copper reduction is severely inhibited, but that the rate of oxidation is enhanced compared to the fresh state of the catalyst. The exact amount of copper accessible for the reaction gases can be quantified by in-situ EPR and it is shown that it decreases by catalyst deactivation and is only partially reclaimed by catalyst regeneration.

[1] D. Nielsen, Q. Gao, T.V.W. Janssens, P.N.R. Vennestrøm, S. Mossin *Cu-speciation in dehydrated CHA zeolites studied by H2-TPR and in situ EPR* J. Phys. Chem. C, 2023, 127(27), 12995-13004
[2] Q. Gao, D. Nielsen, S. Mossin *Dependence of the Al Distribution in CHA Zeolite on the Presence of Na+ during the Synthesis. An EPR Investigation of Cu Species in CuCHA* ChemCatChem, 2024, 16 (4), e202301377
[3] Q. Gao, T. K. Rønne-Nielsen, F. Wen, T.V.W. Janssens, P.N.R. Vennestrøm, S. Mossin, To be submitted

Gäste sind willkommen