Helmholtz - OCPC - Programme 2017-2021

for the Involvement of Postdocs in Bilateral Collaboration Projects with China

PART A

Title of the project
Impact of biodiesel based impurities on exhaust gas after-treatment catalysts

Helmholtz Centre and institute
Karlsruhe Institute of Technology (KIT), Institute for Chemical Technology and Polymer Chemistry (ITCP) and Institute of Catalysis Research and Technology (IKFT)

Project leader
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Description of the project:

A modern diesel engine exhaust gas after-treatment system typically consists of several components: (i) a Diesel Oxidation Catalyst (DOC) used to remove unburned hydrocarbons and CO and to oxidize NO to NO_2, which is beneficial for the following catalytic units, (ii) a Diesel Particulate Filter (DPF) for trapping particulate matter, (iii) a catalyst for selective catalytic reduction of NOx with NH_3 (SCR) and (iv) an Ammonia Slip Catalyst (ASC) for removing excess ammonia leaving the SCR catalyst.[1] The substitution of conventional diesel by biodiesel, presently obtained by transesterification of triglycerides contained in vegetable oils or animal fats, is of high interest due to the limited conventional fuel resources and also of its globally positive impact on pollutant emission.[2] Another strategy is upgraded pyrolysis oil residues.[3] However, alkali and alkaline earth metals, phosphors and sulphur are potential contaminants during such biodiesel application, as they are known to poison the exhaust gas after-treatment catalysts.[2] On the one side, these elements were reported to affect the catalyst surface properties, block the pores by fouling and induce structure collapse or sintering. At the same time, they directly interact with the active sites affecting their electronic and chemical structure, which leads to a significant catalytic activity loss. Particularly the latter aspect is still controversially discussed in literature. This situation is mainly due to the absence of systematic *in situ/operando* investigations, to uncover structure-activity relationships directly under catalytic reaction conditions. Such studies are highly important to comprehensively understand the impact of biodiesel based impurities on exhaust gas after-treatment catalysts and rationally design more robust catalysts.

Within the proposed project we aim at conducting an extensive study on the effect of biodiesel impurities on the activity of Pt-based DOC, V-based SCR catalysts and metal-exchanged zeolite-based SCR catalysts, with the main focus on *in situ/operando* investigations. For this purpose, in addition to conventional material characterisation and catalytic activity tests, advanced *in situ/operando* methods will be used. Essential information on the dynamics in catalyst structure and electronic properties or on the evolution of surface species will be uncovered by studying the catalyst under applied reaction conditions (realistic gas mixture and temperature variations) using Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS), Raman spectroscopy, time and spatially resolved X-ray Absorption Spectroscopy (XAS) and X-ray Emission Spectroscopy (XES). Particularly the new photon-in photon-out technique, such as high energy-resolution fluorescence detected (HERFD) XANES and valence-to-core X-ray emission (v2c XES) spectroscopic methods are expected to provide unique information about the electronic and geometric state and also on active site interaction with different adsorbates for the different fresh and deactivated catalysts.[4,5] To the best of our knowledge, such in-depth investigations have not been reported in literature so far. Their outcome will allow us to accurately identify the effect of biodiesel impurities, and to develop more robust exhaust after treatment catalysts.

The project is based on the excellent expertise of the Grunwaldt group at KIT in DOC-catalysis[6], SCR-catalysis[4,6,7,8], soot oxidation[7] and design of catalysts by novel methods. Furthermore the team is among the world leading groups with extensive experience *in situ/operando* spectroscopy

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using synchrotron radiation.

References:
[1] O. Deutschmann and J.-D. Grunwaldt, *Chem. Ing. Tech.*, 2013, 85, 595. [2] E. Iojoiu, et al., *Emission Control Sci. Technol.*, 2018, 4, 15. [3] P.M. Mortensen, et al., *Appl. Catal. A: Gen.*, 2011, 407, 1. [4] A. Boubnov, et al., *J. Am. Chem. Soc.*, 2014, 136, 13006. [5] D.E. Doronkin, et al., *J. Phys. Chem. C*, 2019, 23, 14338. [6] A.M. Gänzler, et al., *Angew. Chem.Int. Ed.*, 2017, 56, 13078. [7] E. Japke, et al., *Catal. Today*, 2015, 258, 461. [8] L. Zheng, et al., *Top. Catal.*, 2019, 62, 129.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

The collaboration with the Chinese partner, the Dalian Institute of Chemical Physics (DICP), the Chinese Academy of Sciences (CAS) as one of the leading institutes in China, is already well established in the field of catalysis via numerous common projects. The collaboration with DICP, started in 2014, is based on our common interest in catalysis and structure activity relationships ranging from H_2 production and single site catalysis to emission reduction. With mutual benefits, the present collaboration with DICP will deepen the exchange of know-how between the project partners in the field of catalysis and advanced catalyst characterization by *in situ/operando* spectroscopic techniques.

Required qualification of the post-doc:

- PhD in chemistry, chemical engineering, material science or a closely related area;
- Extensive experience in exhaust gas aftertreatment field, catalyst preparation and testing, and *in situ/operando* spectroscopy.
- Besides the professional qualification, strong commitment, independent and self-responsible working including fluent verbal and written English skills are expected. German language skills are a plus.

PART B

Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station in China, which is affiliated to a research institution like a university:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation
- Proof of command of English language

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 35 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team