

# UniCat Colloquium

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### *Tuning of the Nanostructured Metal-Oxide Phase Boundary for Selectivity Control of Methanol Reactions*

Copper-based catalysts are important catalysts in methanol chemistry with use in methanol synthesis from syngas, CO<sub>2</sub> hydrogenation to produce recyclable methanol or methanol steam reforming (MSR). Tunable and reproducible steering of the product selectivity is a prerequisite for technical applications. For MSR the important parameters include high CO<sub>2</sub> selectivity, low CO content and maximum H<sub>2</sub> yield. As for the use of ZrO<sub>2</sub> in the methanol steam reforming reaction, addition of ZrO<sub>2</sub> to Cu/ZnO catalysts allows suppressing the poor sintering stability of the latter. Synergistic Cu-ZrO<sub>2</sub> interactions have similarly been reported for pure Cu/ZrO<sub>2</sub> catalysts, exhibiting direct Cu-O-Zr bonds at the phase boundary. These interactions are considered to play a key role in steering the methanol reforming selectivity to maximum CO<sub>2</sub> yield. A nanocrystalline Cu/tetragonal ZrO<sub>2</sub> catalyst was already reported to be particularly promising in terms of activity, selectivity and stability especially with respect to a technically used Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> methanol synthesis catalyst. Efforts to explain the high selectivity have been considerable and are mainly centered at around two important beneficial parameters: the redox chemistry of Cu at the interface and structural properties within the metallic Cu phase (such as defects or disordered phases).

We have recently reported not only on the structural and chemical steering effects of Cu-ZrO<sub>2</sub> catalysts prepared by different synthesis routines to identify the complex structural prerequisites for CO-, CO<sub>2</sub>- and formaldehyde-selective methanol steam reforming, but also exemplified the surprisingly high activity and extremely high selectivity of a bimetallic Cu/Cu<sub>51</sub>Zr<sub>14</sub> pre-catalyst, in situ decomposed via contact to the MSR reaction mixture. In this case, CO<sub>2</sub>-selective reaction channels were controlled by the resulting Cu-ZrO<sub>2</sub> interface, suppressing full dehydrogenation of methanol to CO and subsequently promoting the total oxidation of intermediate oxygenates to CO<sub>2</sub> by water. The most crucial outcome was the self-activating and self-stabilizing state with co-existence of dispersed Cu and partially hydroxylated tetragonal ZrO<sub>2</sub>, responsible for efficient water activation and, consequently, high CO<sub>2</sub> selectivity.

**Wednesday, November 16, 2016 at 5:15 PM**

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

Building C, Lecture Hall **C 264**

**Prof. Dr. Gurlo (TUB)**

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)

