Inorganic Materials & catalysis

Research Project–Hao Zhang / Nikolay Kosinov / Emiel Hensen

Operando TGA studies of Fe-based catalysts for methane non-oxidative coupling

Background

Due to the large production and low price of methane, it is of great importance to develop effective catalysts for the valorization of natural gas.[1] The activation of methane is difficult because of its high C-H bond strength, negligible electron affinity, and low polarizability. Non-oxidative coupling of methane to C_2 hydrocarbons (ethylene, ethane, and acetylene) is a promising method for its effective utilization.[2] However, this reaction usually occurs at high temperatures (> 900 °C). Developing novel catalysts that can operate under such harsh reaction conditions is very challenging, for example, because of the difficulty in characterizing these systems operando. Recently, we built a ReactorTGA system (TGA: ThermoGravimetric Analyzer), which involves a state-of-the-art magnetic suspension TGA instrument with ultra-high weighting resolution, a gas dosing system, a mass spectrometer, and a gas chromatograph. This apparatus provides us unique opportunities to elucidate the reaction pathways of non-oxidative methane coupling under realistic reaction conditions (**Fig. 1**).

In previous studies, Fe-based catalysts exhibited promising activity and stability in the reaction of non-oxidative methane coupling.[2,3] However, the selectivity to C_2 hydrocarbons needs to be further improved, for which it is desirable to understand the reaction mechanism better. Within this project, you will synthesize a series of Fe-based catalysts and optimize the synthesis conditions. You will test the resulting materials in a new fixed-bed reactor to evaluate their performance. Various modern characterization techniques will be used to investigate the physical and chemical properties of the catalysts with an emphasis on the use of the novel ReactorTGA system to obtain a deep molecular insight into the reaction mechanism and the surface intermediates.

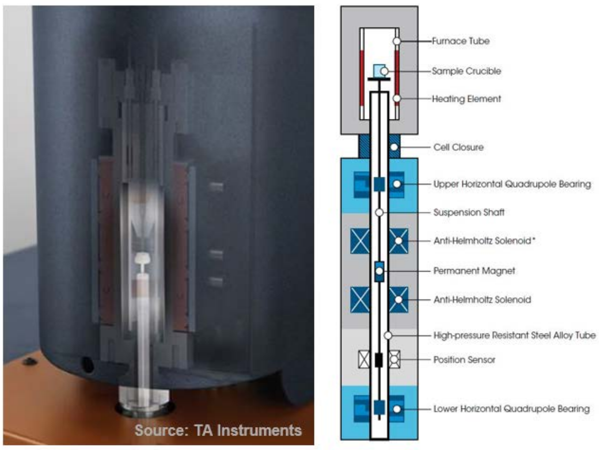

Figure 1. The reaction furnace and configuration of magnetic balance of ReactorTGA system.

Research objectives and techniques:

1. Develop novel Fe-based catalysts with high C_2-hydrocarbon selectivity for methane non-oxidative coupling.
2. Detailed characterization of fresh and used catalysts with X-ray diffraction techniques, X-ray photoelectron spectroscopy, X-ray absorption spectroscopy, and electron microscopy, etc.
3. Investigate structure-activity relations by employing the novel ReactorTGA system under close to real reaction conditions.

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[1] Kosinov et al. *Advanced Materials* 2020, 32, 2202565.
[2] Schwach et al. *Chemical Reviews* 2017, 117, 8497.
[3] Guo et al. *Science* 2014, 344, 616.