FOXSI
Functional Oxide Surfaces and Interfaces

EINLADUNG

zum Vortrag
von

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The application of inelastic neutron scattering to investigate CO hydrogenation over iron based Fischer-Tröpsch synthesis catalysts

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Abstract:

Fischer-Tropsch synthesis (FTS) is making an increasing contribution to hydrocarbon production options; presently, it constitutes a most active area of heterogeneous catalysis research. The reaction may be represented by the following (deceptively) simple chemical equation:

$(2n+1)H_2 + nCO \rightarrow C_nH_{(2n+2)} + nH_2O$.(1)

Recent chemical plant commissions feature unit operations utilising cobalt based catalysts but there remains a significant research interest in iron based FTS catalysts, not least because these materials provide the opportunity for production of valuable unsaturated hydrocarbons [1].

The presentation will concentrate on the surface chemistry surrounding iron based FTS catalysts. This connects with the SFB-FOXSI themes in that, invariably, iron based FTS catalysts are based on iron oxides, which, under FTS conditions, experience a "construction phase" in a process of self-organisation [2]. For example, a hematite precursor compound (α-Fe_2O_3) may be reduced to magnetite (Fe_3O_4), which then reacts to form various carbides [*e.g.* cementite (Fe_3C) and Hägg (Fe_5C_2)]; this combination of structural motifs then defines the active phase of the catalyst [1]. Whereas a variety of conventional analytical techniques are available to characterise such solid-state transformations (*e.g.* Mössbauer spectroscopy, X-ray diffraction, temperature-programmed oxidation, *etc.*), with reference to Equation 1, it is a non-trivial matter to evaluate how hydrogen is partitioned within the catalyst matrix. One technique that is demonstrating increasing application for studying hydrogeneous species in heterogeneous catalysis is inelastic neutron scattering (INS) [3]. In 2013 INS was used for the first time to obtain the vibrational spectrum (50-4000 cm^{-1}) of a commercial grade FTS catalyst extracted from a large-scale coal-to-liquids unit operation (see figure) [4]; with the spectrum establishing a role for a hydrocarbonaceous overlayer in the process chemistry. Follow-up studies using CO hydrogenation as a test reaction over representative iron oxide catalysts suggest that the hydrocarbonaceous overlayer may play an active role in moderating the supply of reagents within the catalyst matrix during the CO dissociative adsorption and CH_x chain propagation processes [5,6]. The presentation will describe how these novel INS measurements are providing new insight in to the operational phase of this economically relevant but complex catalytic system.

FWF SFB F45 „Functional Oxide Surfaces and Interfaces (FOXSI)"
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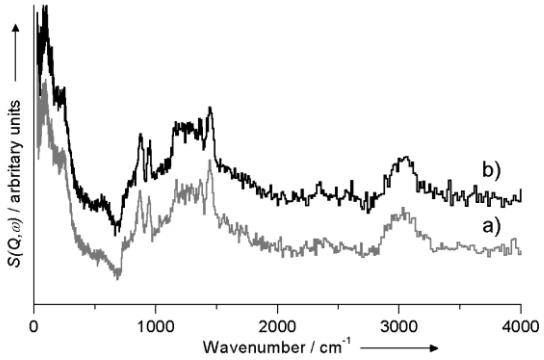

References

[1] J. v. d. Loosdrecht et al., in *Comprehensive Inorganic Chemistry II*; 7 (2013) 525-557, **[2]** H. Schulz, *Topics in Catalysis*, 26 (2003) 1; **[3]** S.F. Parker et al, *Applied Spectroscopy*, 65 (2011) 1325; **[4]** N.G. Hamilton et al., *Angewandte Chemie International Edition,* 52 (2013) 5608; **[5]** N.G. Hamilton et al., *Journal of Catalysis,* 312 (2014) 221; **[6]** R. Warringham et al., *Applied Catalysis A: General,* 489 (2015) 209.

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