Status and Plans for catalysis for sustainable energy

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Renewed interests on olefin production by Fischer Tropsch



 Possible to produce olefin via synthesis gas from natural gas, coal and biomass

Objectives of the project

- The ultimate goal of the project is to identify the principles for rational design of the catalysts to maximize the C₂-C₄ olefin formation and minimize the methane formation from synthesis gas with different hydrogen to CO ratios, by combining competences from NTNU and SJTU
- 1) Preparation of Fe and Co and their alloys with well controlled sizes and surface compositions.
- 2) Correlate chain growth or termination probability to the catalyst properties.
- 3) Apply the gained scientific insights to optimize the catalysts to maximize C₂-C₄ olefin yield.
- 4) Enhance the cooperation between NTNU and SJTU by joint the projects and personal exchanges
- More than 10 joint publications

Status of the project

- Three partner-network has been established for cooperation in the project
- Competences in both groups have been mapped

NTNU

DFT, Kinetics and experiments 2 professor, 1 researcher, 1 PhD

ECUST

SJTU

experiments

DFT, Kinetics and

Coordinator, DFT, Kinetics and

1 PhD, 1 postdoc associated

experiments

1 professor, 1 PhD

Status of the project

- One student has been placed in each group.
 - 2015 January at SJTU (Yu Wang)
 - 2015 September at NTNU (Yalan Wang)
 - 2014 at ECUST (Di Wang, currently visiting NTNU for one year)
- Student exchange
 - The PhD student (Di Wang) from ECUST supported by Chinese scholar council (09.2015-08.2016), 3 months for professor, research stay at NTNU
- The joint project makes it possible to establish a relatively large research groups to combine different competences to carry on cutting-edge research

Status of the project : NTNU

- Microkinetic analysis: predictive modeling
- Catalyst design by microkinetic analysis
- Scaling relationship for adsorption heat and activation energy on different metals

Status of the project (Yu Wang, SJTU)

 Catalyst development of Fe catalysts on Mg-Al spinel support for FTO



Status of the project (ECUST)

- Design and Engineering of Iron-based Composite Catalysts for the Fischer-Tropsch Synthesis of Lower Olefins
- Mechanistic study of F-T synthesis by SSITKA

Catalysts	FeK-OX	FeK-OX+1K	FeK-OX+2K	FeK-OX+5K
CO conversion (%)	28.8	37.6	46.1	60.4
CH selectivity (%C)	70.4	72.2	77	79.5
CH distribution (%C	C)			
CH ₄	19.5	17	16.3	12.9
$C_2^{=}-C_4^{=}$	42.2	43	40.1	35.8
$C_2^{0}-C_4^{0}$	11.4	12.1	10.9	10.2
C ₅₊	26.9	27.9	32.7	41.1
Olefin/Paraffin	3.7	3.6	3.7	3.5

Joint publications

- 1. D. Wang, X. Zhou, J. Ji, X. Duan, G. Qian, X. Zhou, D. Chen, W. Yuan, *Modified* carbon nanotubes by KMnO4 supported iron Fischer-Tropsch catalyst for the direct conversion of syngas to lower olefins, Journal of Materials Chemistry A 3 (2015) 4560-4567.
- 2. D. Wang,, J. Ji, X. Duan, G. Qian, X. Zhou, X. Zhou, D. Chen, *NanoFe catalysts on CNTs for the direct conversion of syngas to lower olefins*, Journal of Energy Chemistry, invited, submitted.
- 3. Yu Wang, Jiachi Chen, Wende Xiao, De Chen, A catalyst for Fischer–Tropsch olefin reaction with MgO modified Al2O3 support. Submitted to The 11th Natural gas conversion symposium, Tomosø, Norway
- 4. Xianzhi Tang, Yu Wang, Wende Xiao, De Chen, *Macroporous* α-Al2O3 support preparation and application in the CO oxidative coupling carbonylation for dimethyl oxalate synthesis, Submitted to The 11th Natural gas conversion symposium, Tomosø, Norway
- 5. Y. Wang, Y. Zhu, Wende Xiao, D. Chen, Mechanism research of of light olefin formation in Fischer-Tropsch synthesis by combination of DFT calculations and microkinetic analysis, Submitted to The 11th Natural gas conversion symposium, Tomosø, Norway
- 6. Xun Huang, Hu Li, De Chen, Wen-De Xiao, Kinetic modeling of the side reactions in methanol-to-olefin process over HZSM-5: an extended study of the previous model, Chem. Eng. J. accepted.

Education

Two departments have agreed to cooperate on the joint education of master students on chemical engineering

- Master students to international master program at NTNU, exchange master students to SJTU
- Master (NTNU) +PhD (SJTU)
- Double degree of master student
- Plan to sign the agreement at kick-off meeting at Beijing

Founding

• Chinese-Norwegian scholarship

Application though Chinese side, and paid by Norwegian Research Council

- Chinese Scholar Council
 - Supporting different scholars: Bachler, master and PhD students, postdoc, researchers and professors (0.5-3 years)