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Wednesday, September 20th, 2023

Clarion Hotel, Somerset 60 Cottontail Lane, Somerset, NJ 08873

Prof. Friederike C. Jentoft



Department of Chemical Engineering University of Massachusetts Amherst

Direct Observation of Transformations and Their Kinetics in Zeolite Pores

Methanol-to-olefins (MTO) conversion is known to proceed via long-lived intermediates in the pores of zeolites or zeotypes, referred to as "hydrocarbon pool" in the literature. The term "pool" illustrates the complexity and the difficulty of determining the exact constitution and the role of these species for formation of select olefins or detrimental coke. Over the past few years, we have established spectroscopic correlations that allow us to identify a variety of hydrocarbon species residing in zeolites pores. These correlations are generally applicable to the analysis of species on the surfaces of solid acids. To gain insight into the reaction steps of MTO, we are monitoring transformations of known, individual pool species. With the help of in situ IR and UV-vis spectroscopy, cyclizations, hydride transfer, ring contraction, and cracking, all of which have relevance in acid catalysis beyond MTO, could be observed. Cyclopentenyl cations have emerged

as an important species in these investigations and serve to determine (i) the role of the volatile precursor for the species formed, (ii) the shape-selectivity of zeolite frameworks for the substitution pattern on the ring after cyclization, (iii) the role of zeolite aluminum content and extra framework aluminum for hydride transfer, and (iv) kinetics. The last two of these examples demonstrate that the spectroscopic data are amenable to quantification and can be used to deliver true activation energies for transformations inside zeolite pores. Therefore, molecular spectroscopies have the potential to deliver deeper insight into the MTO mechanism and other acid-catalyzed reactions and provide guidance on catalyst improvements.

Speaker Bio

Friederike C. Jentoft holds the position of Professor in the Department of Chemical Engineering at the University of Massachusetts Amherst. She studied Chemistry at Eberhard-Karls-Universität Tübingen and at Ludwig-Maximilians-Universität München, where she earned her Dr. rer. nat. (1994) under the guidance of Helmut Knözinger. After working as a postgraduate researcher in Bruce Gates' group at the University of California in Davis, she led a research group in the Department of Inorganic Chemistry for 12 years at the Fritz Haber Institute of the Max Planck Society in Berlin. In 2008, she assumed a faculty position at the University of Oklahoma in Norman, where she was named Anadarko Petroleum Corporation Presidential Professor in 2014. Since 2015, she has been Professor of Chemical Engineering at the University of Massachusetts Amherst. Jentoft received the Award for Young Scientists of the German Society for Petroleum and Coal Science and Technology (1996), a Young Scientists Prize from the International Association of Catalysis Societies (2000), the Excellence in Catalysis Award from the Catalysis Society of Metropolitan New York (2018), and a Lady Davis Fellowship from Technion (2021). From 2009 to 2015, she served as an editor of Advances in Catalysis. Jentoft has authored more than 100 peerreviewed articles and book chapters. Jentoft's research focuses on acid-base catalysis and redox chemistry of Group V-VII metals and capitalizes on her expertise in the spectroscopic analysis of surface reactions. The objective is to make the production of chemicals and monomers more sustainable, by switching to biomass-derived feedstocks, replacing liquid with solid catalysts, and finding substitutes for precious metals. Jentoft has served in various functions for the American Institute of Chemical Engineers, the American Chemical Society, and the North American Catalysis Society. She is a Fellow of the AIChE.

http://che.umass.edu/faculty/friederike-jentoft

ScheduleSocial Hour (Cash Bar)5:30 PMDinner6:30 PMPresentation7:30 PM

Meeting FeesProfessional Members\$40Non-members\$50Students\$25 (Student Members = \$10)Retired/Post-Doc/Unemp.\$40 (Members = \$30)Annual Membership Dues\$35 (Students = \$15)

Deadline for reservations is 12:00PM Tuesday, September 19th, 2023 Please RSVP online using the <u>online form</u>.

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