

ICB seminar series 2015/16

chairman: Prof. Dr. Rudi Gunawan

HALOGEN-MEDIATED PROPANE CONVERSION TO PROPYLENE

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ETH Hönggerberg, 09/09/2015
HCI G 3, 17.00 h

The Seminar will be followed by an Apéro

Abstract. To begin, I will present a short summary of our computational results regarding doped oxides and the role of Lewis acid-base interaction between adsorbates. Then I will switch to the main topic: halogen-mediated oxidative dehydrogenation of an alkane to make an alkene. I will start by presenting the main idea and then show the results of two kinds of experiments. In the first we examined the reaction of propane with oxygen, catalyzed by gas phase I_2 . In the second we reacted propane and oxygen with molten LiI. In both experiments we obtained very high yields of propylene, better than the current “propylene on purpose” industrial processes and better than oxidative dehydrogenation of propane (oxygen plus propane to give propylene and water). In a third set of experiments we showed that reacting oxygen and propane with a molten mixture of LiI and LiBr gives the same propylene yield as the reaction with LiI alone but at much shorter contact time. I will discuss the reaction mechanism and our current understanding of the reasons for the high propylene selectivity.

Speaker highlights. Horia Metiu graduated from Chemical Engineering Department of the Polytechnic Institute in Bucharest in 1961, received his Ph.D. in theoretical chemistry from MIT, in 1974 working with John Ross and Robert Silbey, and then was a postdoctoral fellow at the University of Chicago with Karl Freed. He has been a professor in the Department of Chemistry at the University of California since 1976. In the past he performed theoretical work on surface enhanced spectroscopy, non-adiabatic processes at surfaces, correlation-function theory of rate constants, quantum dynamics with Gaussian wave-packets, spectroscopy in time domain, femtochemistry, genetic programming, crystal growth, thermoelectric materials and polymeric membranes for fuel cells. He has also performed experimental work on Penning spectroscopy of adsorbates, polymeric membranes for fuel cells and mass selected clusters on surfaces. He is currently involved in experimental and computational investigations of catalysis and electrocatalysis.