Strategies for catalyst development: Possibilities of the “rational approach” illustrated with partial oxidation reactions

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The paper discusses two petrochemical selective oxidation reactions namely the practiced formation of styrene (STY) and the desired oxidative functionalistion of propane. The present knowledge about the mode of operation of oxide catalysts is critically considered. The dehydrogenation of ethylbenzene (EB) should be described by an oxidehydration with water actig as oxidant. The potential role of the coke formed during catalytic reaction as co-catalyst will be discussed. Selective oxidation is connected with participation of lattice oxygen mechanism which transforms unselective gas phase oxygen into selective oxygen. The atomistic description of this process is still quite unclear as well as the electronical structural properties of the activated oxygen atom. The role of solid state acidity as compared to the role of lattice oxygen is much less well investigated modem multiphase-multielement oxide (MMO) catalysts. The rational is that the significant efforts made to improve current MMO systems by chemical modifications can be very much more fruitful when in a first step the mode of action of a catalyst is clarified on the basis of suitable experiments. Such time-consuming experiments at the beginning of a campaign for catalyst improvement pay back their investment in later stages of the project when strategies of chemical development can be derived on grounds of understanding.