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Towards the Unravelling of Catalytic Reaction Kinetics: Styrene Synthesis over Iron Oxide Catalysts

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Despite decades of investigations into the catalytic dehydrogenation of ethylbenzene to styrene, the mechanism of this important industrial reaction is still largely unknown. Recently, we succeeded in growing iron oxide films epitactically onto platinu m single crystals, producing well defined model catalysts as characterised by LEED and STM. The catalytic activity of these films was investigated in a single -crystal flow-reactor (p= 5 - 50 mbar) and closely reflected the behavior of the industrial cataly sts: Fe3O4 is inactive, Fe2O3 shows low and K-promoted FexOy high activity. Furthermore, active catalysts show activation periods which are accompanied by increasing surface disorder. Based on these experiments, we are developing an elementary-step kinetics, which allows a testing of mechanistic assumptions and a discrimination between different kinetic models through a comparison between simulations and experiments. We thus aim at developing a methodology for the derivation of reliable catalytic reaction kinetics through an integrated experimental and model -based approach.