



*Time-resolved studies on correlations between dynamic electronic structure and selectivity of a  $H_5[PV_2Mo_{10}O_{40}]$  partial oxidation catalyst*

*Ressler, T.<sup>\*1</sup>; Timpe, O.<sup>2</sup>*

*1 Technical University Berlin*

*2 Fritz-Haber-Institut*

*\* corresponding author*



Abstract

Time-resolved in situ X-ray absorption spectroscopy studies on an activated  $H_5[PV_2Mo_{10}O_{40}]$  oxidation catalyst were performed to obtain correlations between the dynamic structure and the catalytic selectivity of the material. Both the geometric and the electronic structure of the vanadium and molybdenum metal centers of the catalyst change dynamically under the reaction conditions employed. Moreover, the selectivity of the catalyst exhibited a pronounced correlation with the degree of reduction and the solid-state kinetics of the re-oxidation process. The corresponding extent of re-oxidation curve could be simulated with a solid-state kinetic model assuming three-dimensional diffusion as rate-limiting step. Hence, the partially reduced catalyst exhibited a rate constant of the bulk-diffusion limited re-oxidation which coincided with the temporal evolution of the selectivity of the catalyst.