Investigating the Surface Termination Effect of $CoFe_2O_4$ on the Selectivity in the Catalytic 2-Propanol Oxidation via ME-DRIFTS and RAMAN Spectroscopy

<u>Nicolas Cosanne¹</u>, Wilma Busser², Anna Rabe³, Malte Behrens¹, Martin Muhler², Sharif Najafishirtari¹

¹Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany ²Ruhr-Universität Bochum, 44801 Bochum, Germany ³University of Duisburg-Essen, 45141 Essen

E-Mail presenting author: ncosanne@ac.uni-kiel.de

Phase-pure isotropic and anisotropic CoFe₂O₄ nanoparticles were synthesised with the desired morphology.[1] A {111} termination for the anisotropic platelets is assumed.[1] Both catalysts were tested in the gas-phase 2-propanol oxidation. While the anisotropic catalyst displayed low propene selectivity of less than 5% and high acetone selectivity, the isotropic catalyst had 28% selectivity towards propene in the dry feed (see Figure 1a). The selectivity was not impacted by the presence of water in the gas-feed. To further analyse the differences between both catalysts in the dry and wet feed, activation energies and reaction orders were determined, which also revealed that the {111} surface was more impacted by gas-phase water. Furthermore, ME-DRIFTS (Figure 1b and 1c) and RAMAN measurements have been conducted to probe the (surface) properties of both catalysts. The selectivity changes can be attributed to different acid-base properties of the exposed surfaces, since more acidic sites favour propene formation. The ME-DRIFTS results also show different OH and acetate surface species on both catalysts.

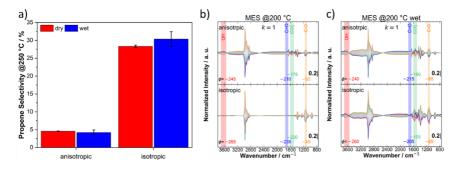


Figure 1: Propene selectivity (a) and ME-DRIFTS spectra of $CoFe_2O_4$ catalysts under dry (b) and wet (b) feed conditions.

A. Rabe *et al, Chem. Eur. J.*, **2021**, 27, 17038-17048, 10.1002/chem.202102400
S. Anke *et al, ACS Catal.*, **2019**, 9, 7, 5974–5985, 10.1021/acscatal.9b01048