



	Experiment title: ZnO-Al ₂ O ₃ catalysts for propane dehydrogenation: correlating structure with catalytic performance	Experiment number: A31-1-60
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Report: Abstract

We correlate the catalytic activity for propane dehydrogenation (PDH) of a series of Zn-based Al₂O₃ catalysts with their structure and structural evolution. To this end, three model catalysts are investigated: (i) ZnO/Al₂O₃ prepared by atomic layer deposition (ALD) of ZnO onto γ -Al₂O₃ followed by calcination at 700 °C, which yields a core-shell spinel zinc aluminate/ γ -Al₂O₃; (ii) zinc aluminate spinel nanoparticles (Zn_xAl_yO₄ NPs) prepared via a hydrothermal method; and (iii) ZnO/SiO₂ prepared by ALD of ZnO on SiO₂. The catalysts are characterized by synchrotron X-ray powder diffraction (XRD), Zn K-edge X-ray absorption spectroscopy (XAS), and ²⁷Al solid-state nuclear magnetic resonance (ssNMR). We identify tetrahedral Zn sites in close proximity to Al sites of a zinc aluminate spinel phase (Zn_{IV}-O-Al_{IV/VI} linkages) as more active and selective in PDH relative to the supported ZnO wurtzite phase (Zn_{IV}-O-Zn_{IV} linkages) in ZnO/SiO₂. 50ZnO/Al₂O₃ gives 77% selectivity to propene at 9 mmol C₃H₆ g_{cat}⁻¹ h⁻¹ space-time yield after 3 min of reaction at 600 °C. The ZnO/Al₂O₃ catalyst shows an

irreversible loss of activity over repeated PDH and air-regeneration cycles attributed to Zn depletion on the surface, while the activity loss of $Zn_xAl_yO_4$ NPs due to coke deposition can be recovered by air regeneration.¹

1. Nadjafi, M.; Kierzkowska, A. M.; Armutlulu, A.; Verel, R.; Fedorov, A.; Abdala, P. M.; Müller, C. R., Correlating the Structural Evolution of ZnO/Al₂O₃ to Spinel Zinc Aluminate with its Catalytic Performance in Propane Dehydrogenation. *Journal of Physical Chemistry C* **2021**, *125* (25), 14065-14074.