Supporting Information

Niobia as an efficient catalyst for the epoxidation of dicyclopentadiene

Sang-Ho Chung,[1] Vikash Lachman,[1] Thierry Slot,[1] N. Raveendran Shiju[1*]

[1] Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, P.O. Box 94157, Science Park, 1098 XH Amsterdam, The Netherlands.

[*] E-mail: (N.R.S.) n.r.shiju@uva.nl

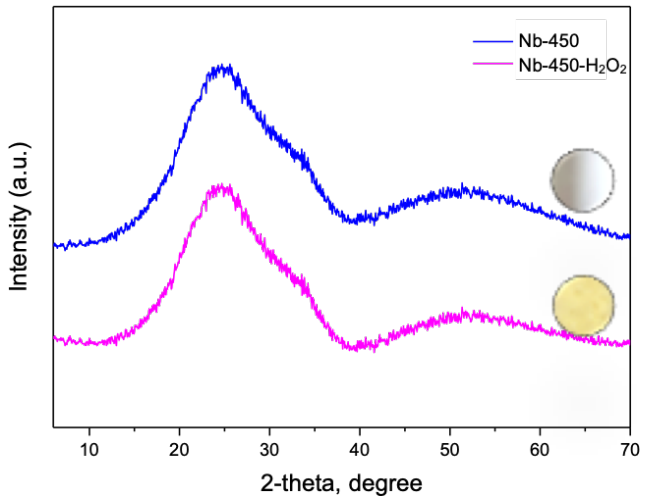

Figure S1. Powder X–ray diffraction patterns of Nb–450 and Nb–450–H_2O_2 with the observed color of the catalysts.

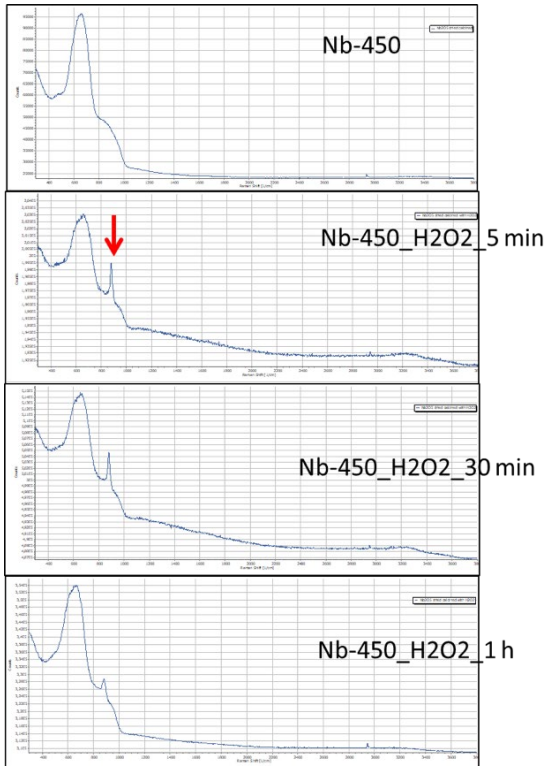

Figure S2. Raman spectra of Nb–450 after H_2O_2 treatment at different measurement times.

Catalyst reuse study. The Fig. S3 shows the results of catalytic reusability studies for Nb–450 and Nb–450–H_2O_2. The catalysts were dried at 60 °C and calcined at 220 °C for 2 h before recycling. A decrease in the conversion of DCPD was observed (90, 51, 21 and 15% for each recycle test at 1 h of reaction time). After the 1st recycle, no lag phase was observed for each run, indicating that the catalyst did not lose (all of) the peroxo species on Nb–450–H_2O_2 catalyst. In Fig. S3b, the product distribution showed favorable formation of P2 than P1 after each recycle, compared at the same DCPD conversion (10%). XRD analysis showed that the crystalline TT–phase was formed after each recycle tests (Fig. S5). Furthermore, the intense yellow color of Nb–450–H_2O_2 became grey–brown, suggesting the formation of coke on the catalyst surface. After the third recycle test, an IR band was observed at around 1400 cm^{-1}, showing the ethylene-type carbonaceous materials (Fig. S5) [1].

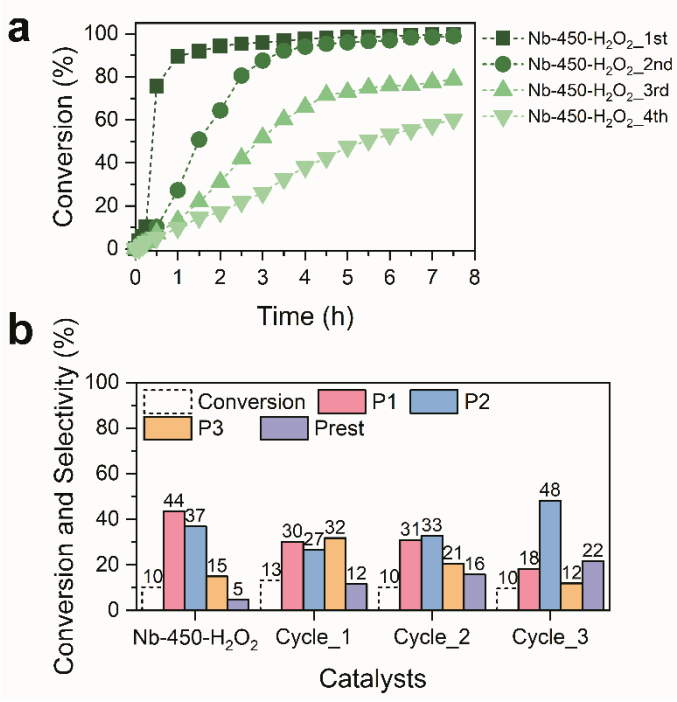

Figure S3. Conversion and selectivity to DCPD epoxides during catalyst recycle tests. Reaction conditions: acetonitrile (49 mL), DCPD (1.3 mL), Nb_2O_5–450 (150 mg), H_2O_2 (4.3 mL) at 60 °C. After each cycle, the catalysts were dried at 60 °C and calcined at 220 °C for 2 h before recycling.

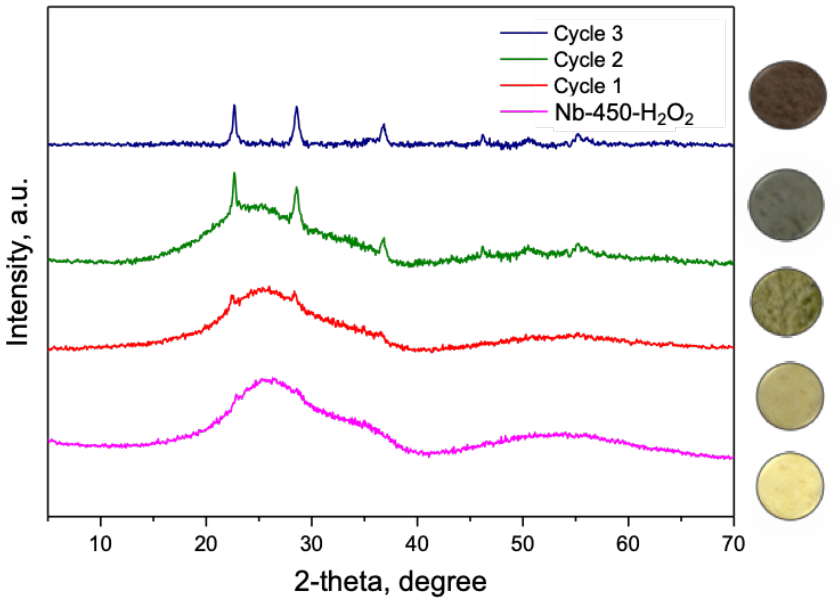

Figure S4. Powder X–ray diffraction patterns of Nb–450–H_2O_2 with the observed color of the catalysts after recycling tests.

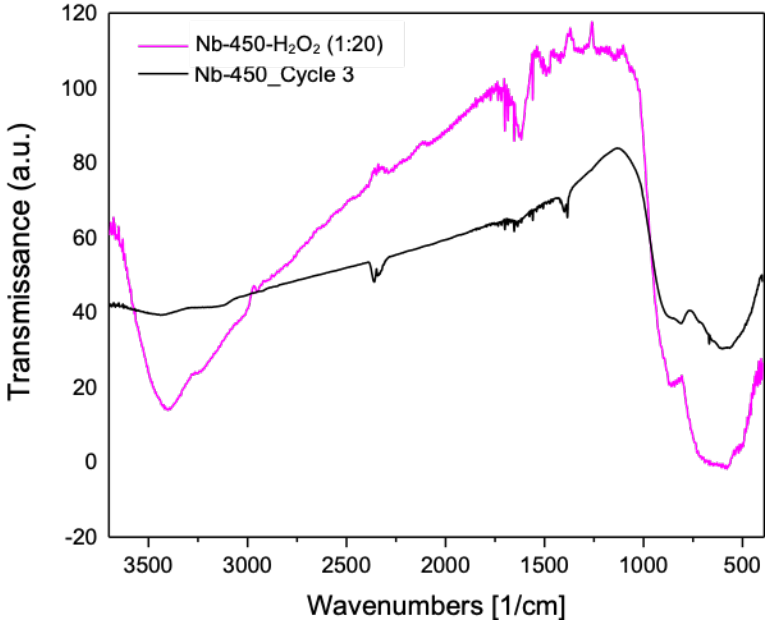

Figure S5. FT–IR spectra of Nb–450–H_2O_2 after recycling tests.

References

[1] H.G. Karge, W. Nießen, H. Bludau, In-situ FTIR measurements of diffusion in coking zeolite catalysts, Appl. Catal. A Gen. 146 (1996) 339–349. https://doi.org/10.1016/S0926-860X(96)00175-5.