Electronic Supplementary Information
Towards sustainable manufacture of epichlorohydrin from glycerol using hydrotalcite-derived basic oxides

Giacomo M. Lari, Giorgio Pastore, Cecilia Mondelli* and Javier Pérez-Ramírez*

Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland.
E-mail addresses: cecilia.mondelli@chem.ethz.ch; jpr@chem.ethz.ch

Table S1. Characterisation data of the materials evaluated in the dehydrochlorination of dichloropropanol.

Sample	V_{pore} [a] / cm^3 g^{-1}	S_{BET} [b] / m^2 g^{-1}	C_B [c] / μmol g^{-1}	C_A [d] / μmol g^{-1}	C [e] / wt.%
MgO	0.45	482	364	6	3.0
USY	0.53	648	0	58	8.4
USY-AT	0.49	600	184	12	2.1
γ-Al_2O_3	0.50	85	5	85	5.6
MgO/USY	0.51	612	181	68	5.0
Y	0.48	680	19	221	5.2
Y-AT	0.27	406	389	161	4.1

[a] Volume of N_2 adsorbed at $p/p_0 = 0.98$. [b] Total surface area, BET method. [c] Concentration of basic sites, CO_2-TPD. [d] Concentration of acid sites, FTIR spectroscopy of adsorbed pyridine. [e] Carbon content, elemental analysis.

Table S2. Activity and selectivity data of the materials evaluated in the dehydrochlorination of dichloropropanol.

Sample	$X_{dichloropropanol}$ / %	$S_{epichlorohydrin}$ / %	$S_{chloroacetone}$ / %	S_{others} / %
MgO[a]	5.5	31.6	12.1	14.0
USY[a]	1.2	1.2	26.3	30.0
USY-AT[a]	2.2	23.4	15.5	18.8
γ-Al_2O_3[a]	0.8	33.3	13.8	16.9
MgO/USY[a]	3.7	62.1	18.5	18.9
Y[a]	0.1	0.5	15.1	16.4
Y-AT[a]	5.0	57.2	14.6	15.6
HT2[a]	5.9	74.3	15.7	18.0
HT2-c823[a]	7.8	80.5	18.9	20.1
HT2[b]	6.1	75.5	4.8	10.0
HT4[b]	5.3	70.7	9.3	8.9
HT2-c823[b]	7.9	79.6	3.2	7.5
HT4-c673[b]	1.9	68.2	8.3	14.1
HT4-c823[b]	18.2	94.8	2.7	2.6
HT4-c973[b]	5.9	80.8	6.1	12.5

[a] $T = 473$ K, $P = 1$ bar, $t = 0.5$ h and $WHSV = 6$ h^{-1}. [b] $T = 423$ K, $P = 1$ bar, $t = 0.5$ h and $WHSV = 6$ h^{-1}.

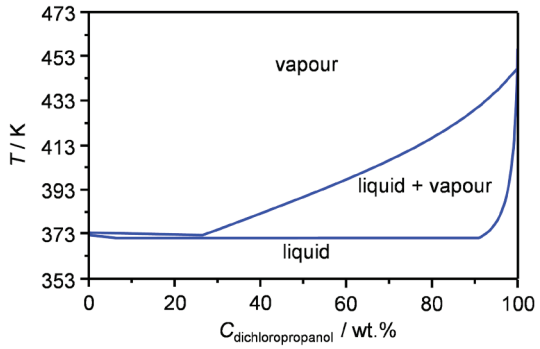

Fig. S1. Liquid-vapour equilibrium diagram for the 1,3-dichloropropanol-water mixture at 1 bar.

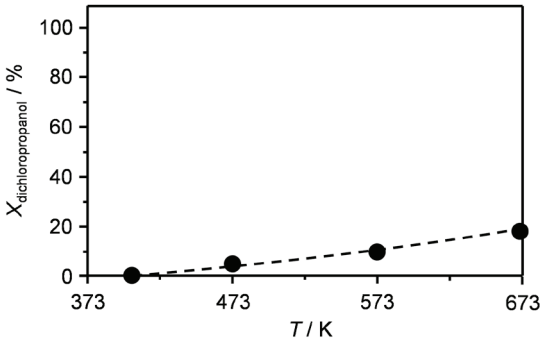

Fig. S2. Dichloropropanol conversion *versus* temperature in experiments conducted in the absence of any additional reagent at $P = 1$ bar and $WHSV = 1.2\ h^{-1}$.

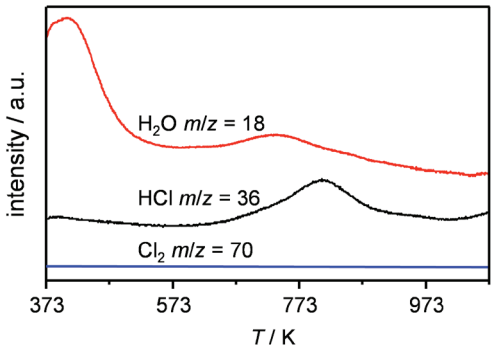

Fig. S3. Mass spectrometry analysis of the outlet gas upon the temperature-programmed oxidation (O_2 concentration in He = 10 vol.%, ramp rate = 10 K min^{-1}) of the HT4-c823 material after use in the dehydrochlorination of dichloropropanol.

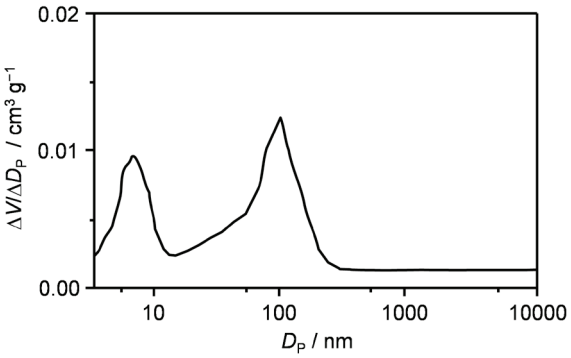

Fig. S4. Pore size distribution of HT4-c823 derived from the adsorption branch of the N_2 sorption isotherm through the application of the BJH model.