Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

SI: Surface chemistry of MgO/SiO_2 catalysts during the ethanol catalytic conversion to 1,3-butadiene: *in situ* DRIFTS and DFT study

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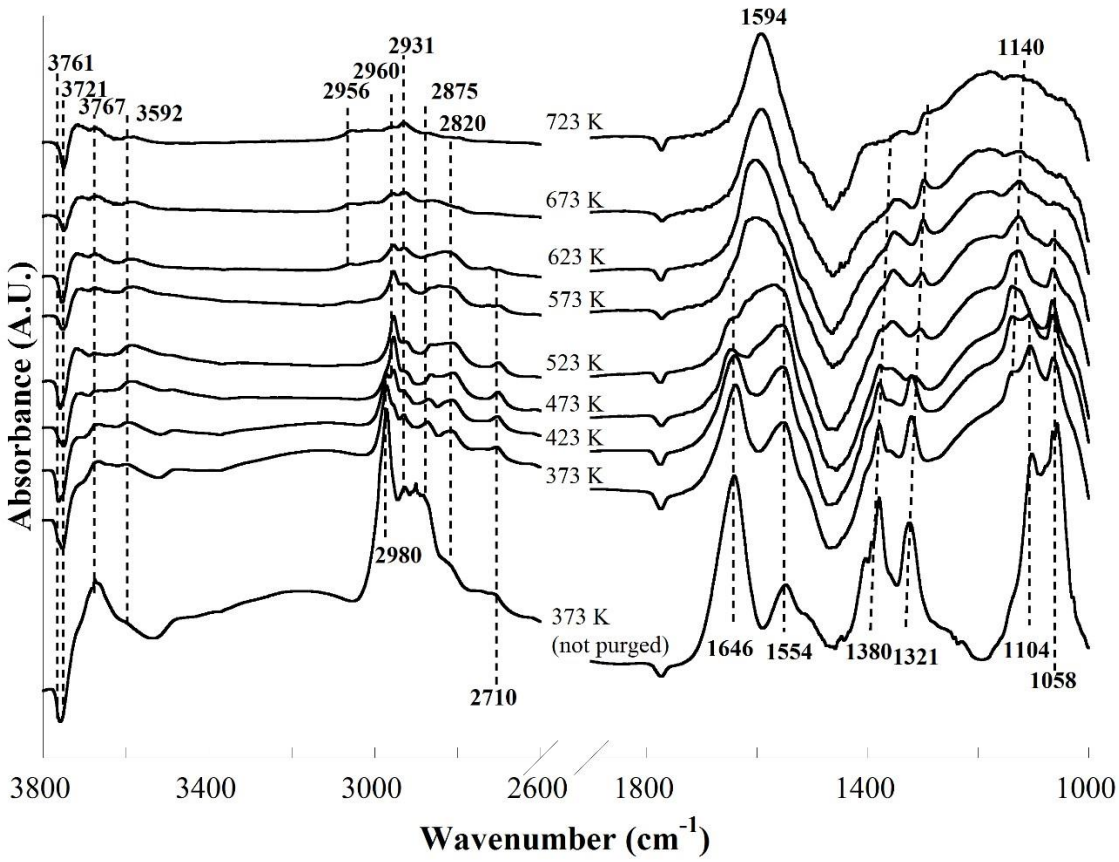

Figure S1. *In-situ* spectroscopy of ethanol on MgO catalyst. Ethanol was adsorbed on the sample surface and temperature ramped up from 373 to 723 K while spectra being recorded. Subtracted spectra are shown. Spectra are offset for clarity.

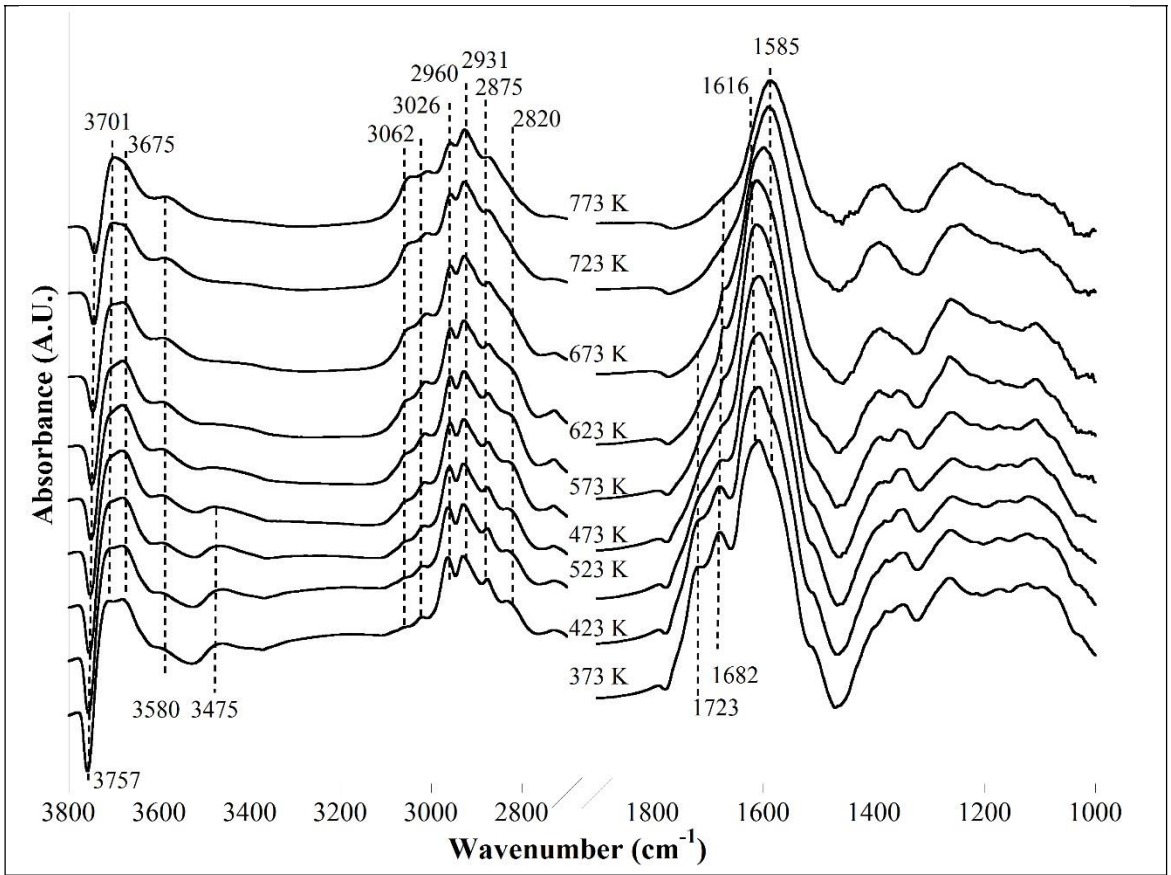

Figure S2. *In-situ* spectroscopy of acetaldehyde on MgO catalyst. Acetaldehyde was adsorbed on the sample surface and temperature ramped up from 373 to 723 K while spectra are being recorded. Spectra are offset for clarity.

Table S1. Calculated infrared frequencies of gas phase ethanol, acetaldehyde, crotyl alcohol and crotonaldehyde molecules. Frequencies were calculated using PBE density functional and no scaling to correct for anharmonicity was applied. Experimental frequencies, except for crotonaldehyde, were obtained from NIST.[68]

Vibration	Ethanol		Acetaldehyde		Crotyl alcohol		Crotonaldehyde	
	DFT Frequency (cm^{-1})	IR (cm^{-1})	DFT Frequency (cm^{-1})	IR (cm^{-1})	DFT Frequency (cm^{-1})	IR (cm^{-1})	DFT Frequency (cm^{-1})	IR (cm^{-1})
ν (OH)	3718	3686	-	-	3702	3665	-	-
ν CH_3	3053, 3038, 2966	3035, 3012, 2960	3092, 3025, 2967	3024, 2996, 2967	3008, 2959	2970	3068, 3011, 2965,	2984
ν CH_2	3011, 2925	3008, 2905	-	-	3000, 2928	2940, 2880	-	-
ν CH	-	-	2790	2840	3062, 3055, 3037	3030	3095, 3065, 3042, 2788	3044, 3007, 2750, 2828
ν (C=O)	-	-	1749	1743	-	-	1691	1693
ν (C=C)	-	-	-	-	1675	1675	1644	1645
δ (CH_2, CH_3)	1463	1456	1413, 1406	1410, 1390	1448, 1439, 1425, 1359	1480, 1435, 1415, 1338	1430, 1420, 1353	1449, 1398, 1381
δ (OH)	1325	1391	-	-	-	-	-	-
δ (COH)	-	-	-	-	-	-	1367	Not observed
δ (CCH)	1237	1242	-	-	-	-	1288	Not observed
Combination bending	-	-	-	-	1362, 1313, 1285, 1261, 1170, 1115, 1024	1384, 1290, 1250, 1180	1236	Not observed

Combination stretch	-	-	-	-	1075	1080	1142, 1086	1151, 1082
ν (CO)	1027	-	-	-	981	970	-	-
ν C-C (C=C)	863	-	1095	1122	-	-	-	-
Scaling factor	**0.997**		**0.9962**		**0.9903**		**0.9996**	