Ga/HZSM-5 catalysed acetic acid ketonisation for upgrading of biomass pyrolysis vapours

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catalysts

MDPI

Supplementary Materials

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Characterisation

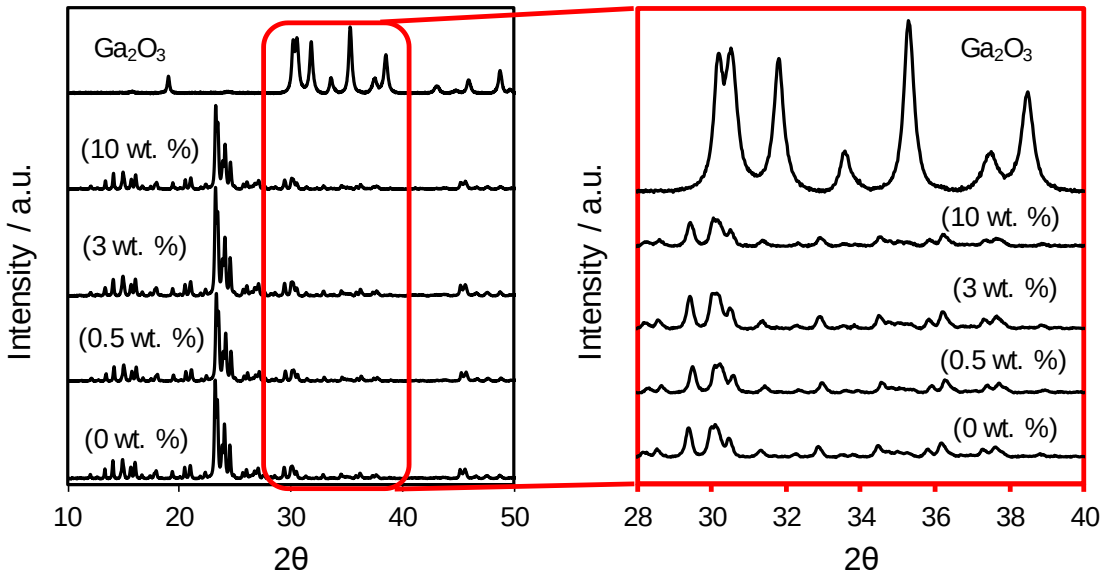

Figure S1. XRD patterns of xGa/HZSM-5 and bulk Ga_2O_3.

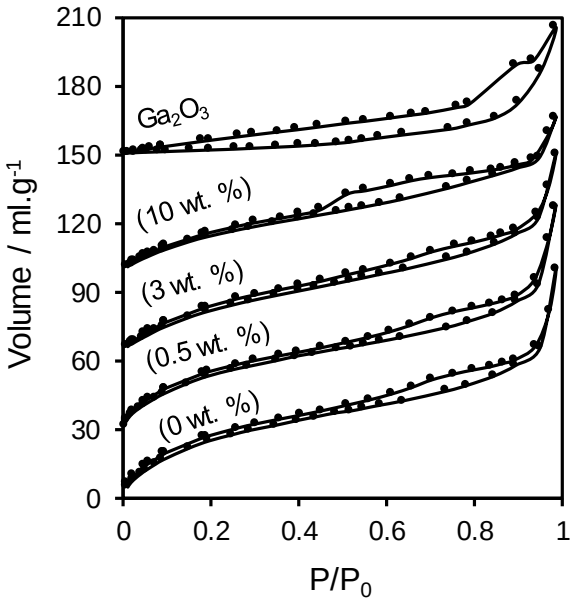

Figure S2. N_2 adsorption-desorption isotherms of xGa/HZSM-5 and G_2O_3.

Table S1. Surface and bulk compositions of xGa/HZSM-5 and Ga_2O_3.

Catalysts	Surface composition (XPS)				Bulk composition (ICP)
	O / wt%	Si / wt%	Al / wt%	Ga / wt%	Ga / wt%
HZSM-5	46.9	50.1	3.0	0	0
0.5Ga/HZSM-5	47.1	50.2	2.5	0.2	0.3
3Ga/HZSM-5	47.5	49.5	2.7	0.3	3
10Ga/HZSM-5	40.3	50.6	3.0	6.1	9
Ga_2O_3	37.1	0	0	62.9	75

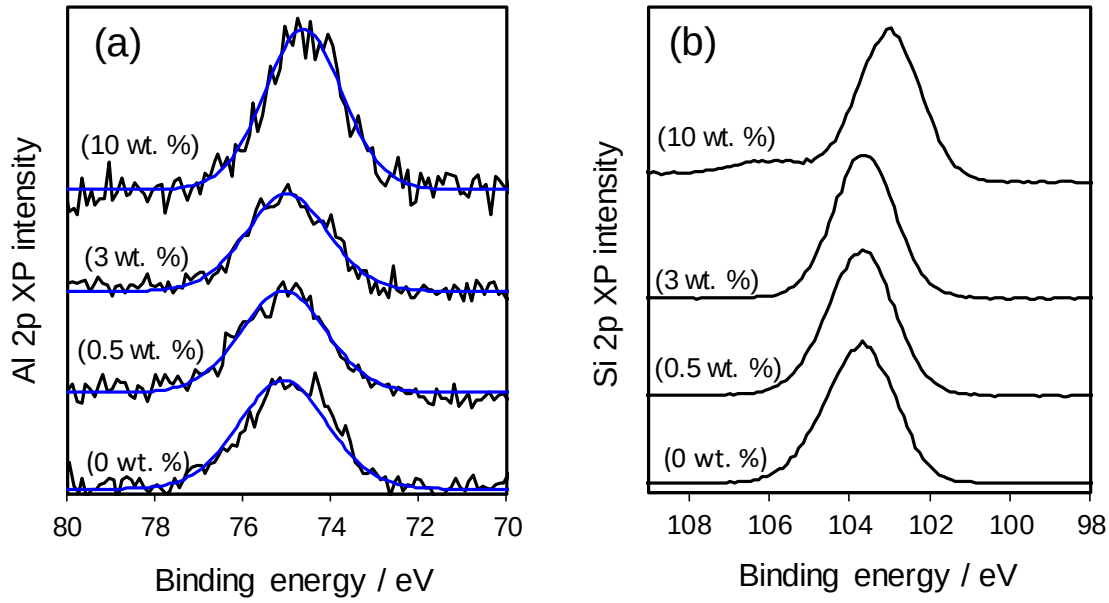

Figure S3. (a) Al and (b) Si 2p XP spectra of xGa/HZSM-5.

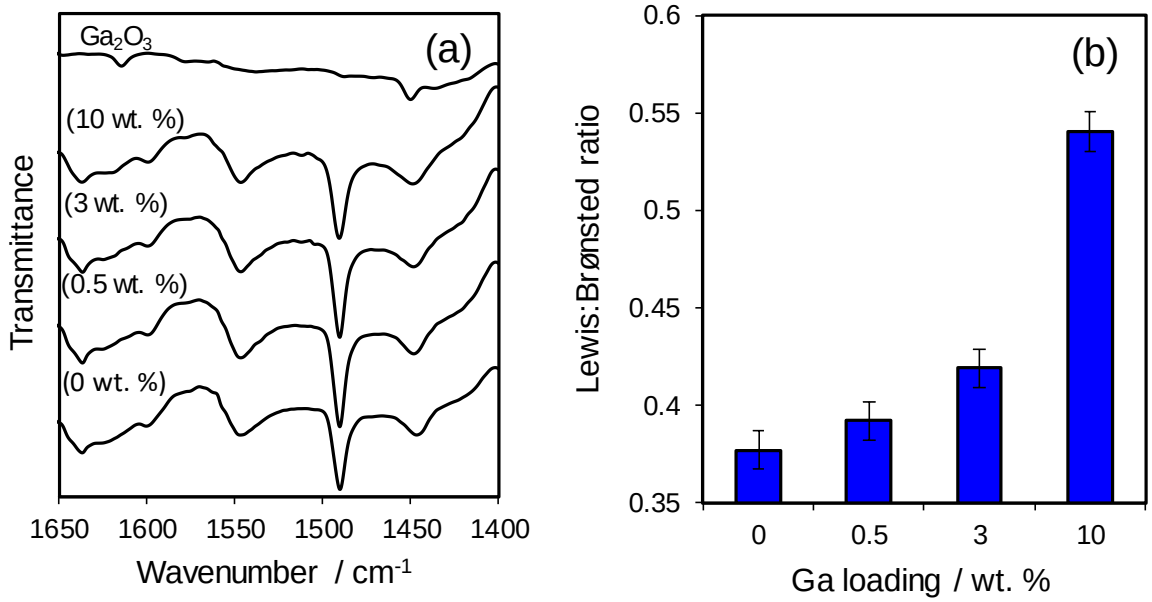

Figure S1. (a) DRIFT spectra of pyridine-saturated xGa/HZSM-5 and Ga_2O_3 and (b) corresponding Lewis:Brønsted acid site ratio (1444 cm^{-1}:1545 cm^{-1} bands) for xGa/HZSM-5.

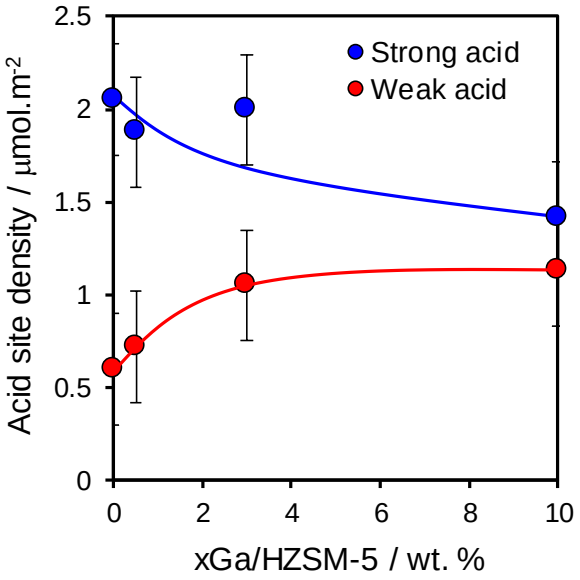

Figure S5. Density of strong and weak acid sites for xGa/HZSM-5 from propylamine TPRS.

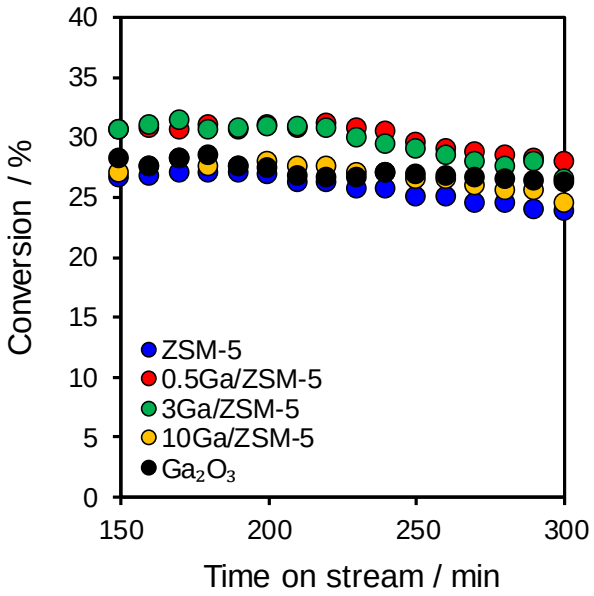

Figure S2. Acetic acid conversion over xGa/HZSM-5, and Ga_2O_3 vs time on stream. Reaction conditions: 200 mg catalyst, at 400 °C, 0.2 mL.min^{-1} acetic acid, 50 mL.min^{-1} N_2, 1 bar.

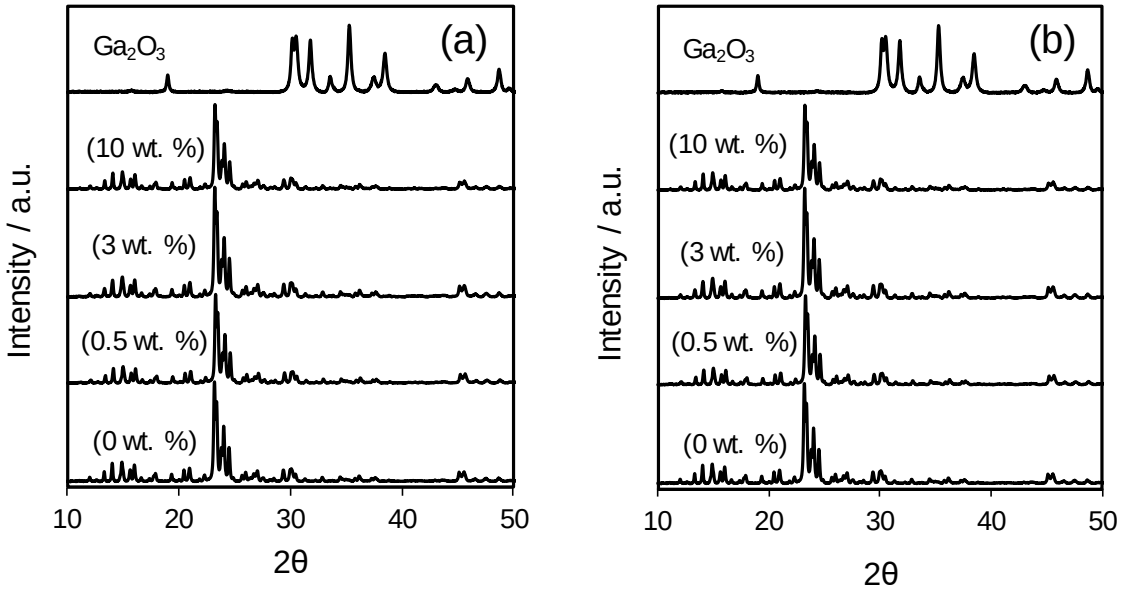

Figure S7. XRD patterns of (a) fresh and (b) post-reaction xGa/HZSM-5 and Ga_2O_3.

Table S2. Post-reaction carbon content of xGa/HZSM-5 and Ga_2O_3 after 5 h acetic acid ketonisation at 400 °C.

Catalyst	Carbon content[a] / wt%
HZSM-5	12.0
0.5Ga/HZSM-5	11.8
3Ga/HZSM-5	12.1
10Ga/HZSM-5	11.9
Ga_2O_3	1

[a] CHNS analysis.

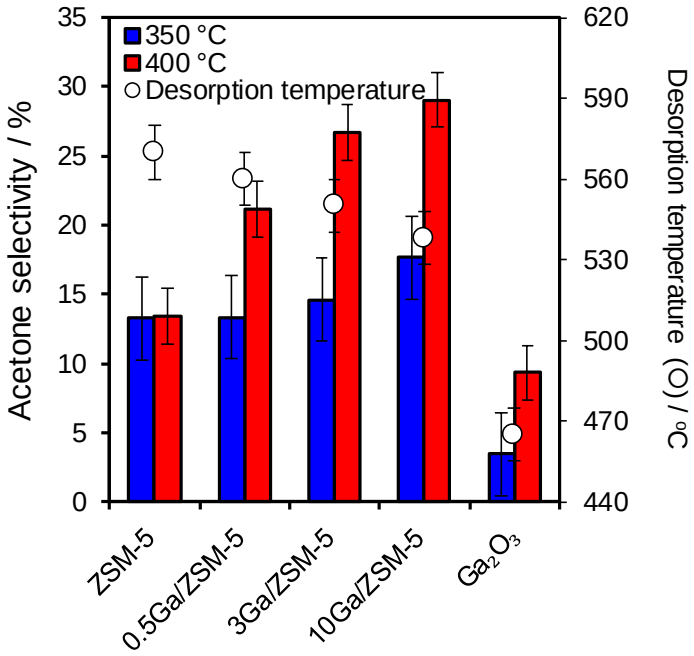

Figure S8. Correlation between acetone selectivity from acetic acid ketonisation at iso-conversion (23 % and 29 % at 350 °C and 400 °C , respectively) and acid strength from propylamine temperature-programmed reaction spectroscopy over xGa/HZSM-5, and Ga_2O_3. Higher temperatures indicate weaker acidity; the maximum propene desorption temperature from weak acid sites in Figure 4 is shown.