Electronic Supplementary Material (ESI) for ChemComm.

A facile and sustainable one-pot approach to the aqueous and low-temperature PET-to-UiO-66(Zr) upcycling

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Experimental

FTIR spectra were acquired using an attenuated total reflectance (ATR) setup using a Bruker Tensor 27 spectrometer. A resolution of 4 cm^{-1} was used with a range of 400-4,000 cm^{-1}, with 32 scans using the OPUS software package.

X-ray photoelectron spectra were acquired under ultrahigh vacuum (<5×10^{-7} Pa) on a Thermo Fisher Nexsa XPS System with a monochromated Al K-alpha X-ray source (photon energy = 1486.7 eV). A pass energy of 50 eV was used with a flood gun as an electron source for charge neutralisation. The data was analysed using the OriginPro software. Peaks were fitted with a Gaussian numerical convolution after baseline and background corrections.

PXRD data was collected on a Panalytical X'Pert Pro in reflection mode using a Cu K_α anode (λ = 1.54178 Å), divergence slit, Ni-filter and a range of 5-120° 2Θ.

The N_2 adsorption isotherms were obtained at 77 K using a Tristar II Plus Micromeritics equipment. The specific surface areas were calculated with the multipoint Brunauer–Emmett–Teller (BET) method and pore size distributions (PSD) were obtained using a non-local density functional theory (NLDFT) model from the adsorption line of the isotherm.

Thermal Gravimetric analysis was performed using a Pyris-PerkinElmer TGA 8000 instrument under air atmosphere, at 10 °C min^{-1} in the 30 - 900 °C range.

Differential Scanning Calorimetry was carried out on a PerkinElmer LAMBDA™ 365 at a heating rate of 50 °C min^{-1} between 20 and 270 °C.

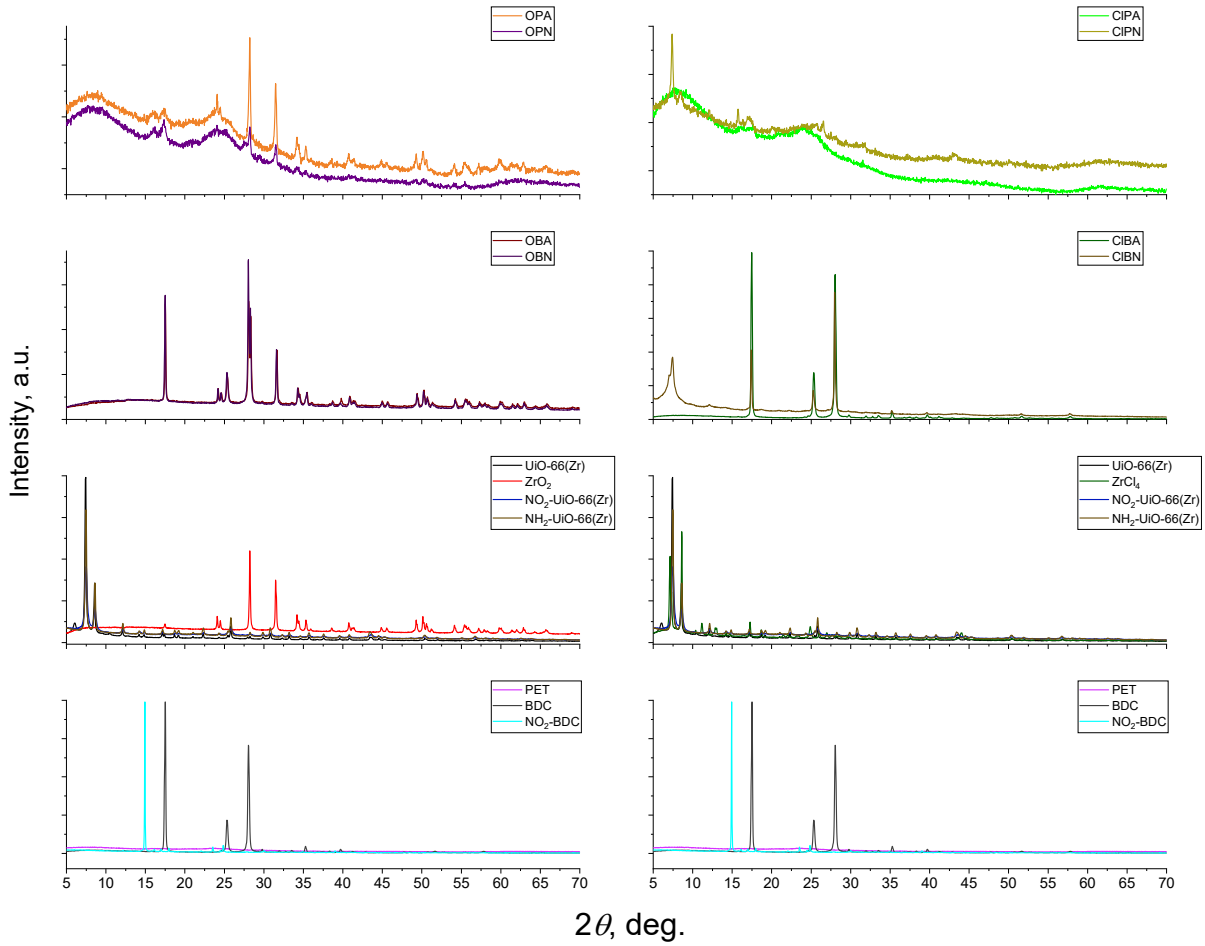

Figure S1 *PXRD traces for the various reaction mixtures and reference materials*

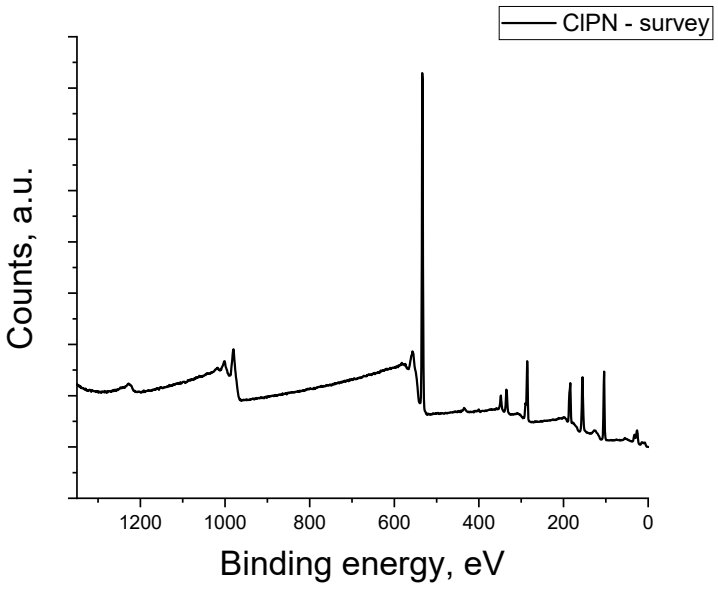

Figure S2 *XPS survey spectrum for the ClPN sample*

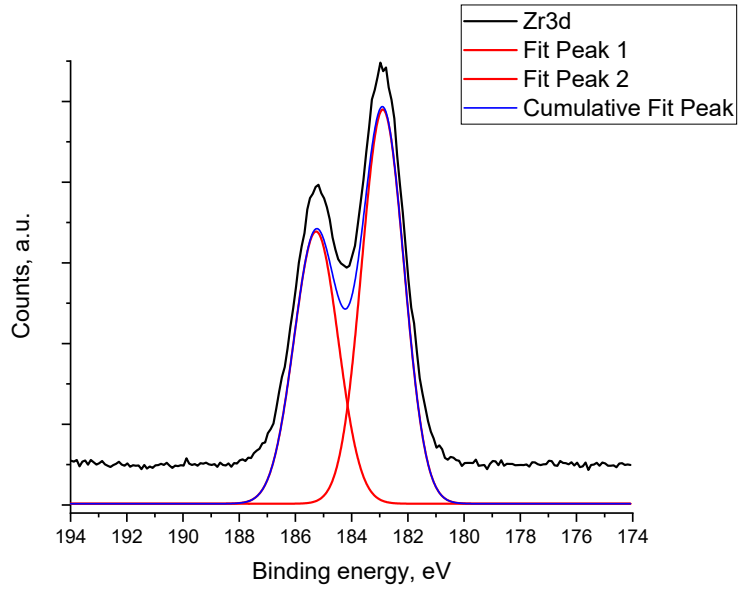

Figure S3 *High-resolution Zr3d ZPS spectrum for ClPN*

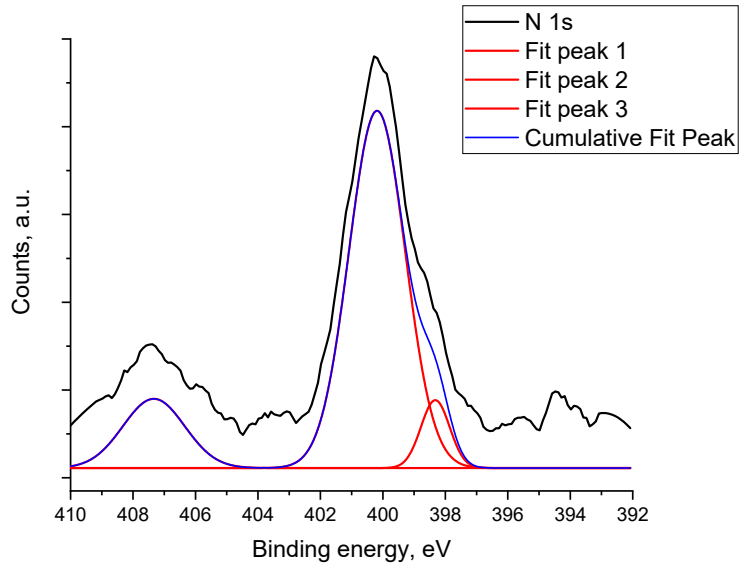

Figure S4 *High-resolution N1s spectrum for ClPN*

Table S1 *Binding energies as obtained from fitting the XPS spectra*

XPS peak assignment	XPS peak position, [eV]	Fitted peak areas / proportion
Zr $3d_{3/2}$	185.3	
Zr $3d_{5/2}$	182.9	
N 1s (-NO_2 groups)	407.3	0.391 / 16.2%
N 1s (-NH_2 groups)	400.2	1.849 / 76.4%
N 1s (-NH_2 groups)	398.3	0.178 / 7.4%

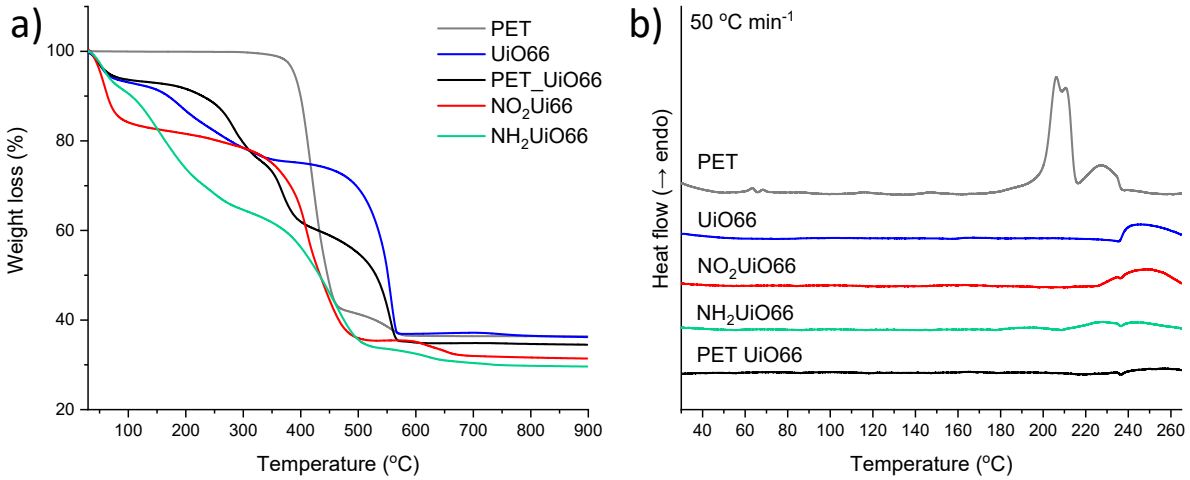

Figure S5 *Thermal gravimetric analysis (a) and Differential Scanning Calorimetry data (b) of PET-derived MOF and reference materials*