Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information for

A visually detectable pH responsive zirconium metal-organic framework

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Experimental Section

Instrumentation

NMR spectra for hydrolysis profiles of simulant were collected on a 400 MHz Agilent DD MR-400 at IMSERC (Integrated Molecular Structure Education and Research Center) of Northwestern University. Nitrogen isotherm measurements were carried out on a Micromeritics Tristar Ⅱ 3020 at 77K. Samples were activated at 150 ^{0}C under vacuum for 12 h. UV-Vis spectra were collected on a Cary 5000 spectrophotometer in dual beam mode. Scanning electron microscopy images were collected on a Hitachi S-4800-II. The sample was coated with osmium tetroxide (9 nm) using sputter before using SEM.

Synthesis of NU-1000-CNF by SALI

NU-1000 was made according to a recently published modified procedure.[1] 23 mg of NU-1000 (0.011 mmol) was added to 4-dram vial with 2 mL of DMF and 25 mg of 5(6)-carboxlynaphtofluorescein (CNF)(0.053 mmol) which was purchased from Sigma-Aldrich. After sonication for 5 min, the mixutre was heated at 80 ^{0}C for 24 h. After cooling to room temperature, the solution was removed and the material was washed twice with DMF to remove the residual CNF. Subsequently the solid residue was washed twice with acetone and NU-1000-CNF was filtered and dried at 80^{0}C under vacuum for 12h.

Hydrolysis experiment with DMNP

Hydrolysis profiles were recorded by in-situ ^{31}P NMR spectroscopy at room temperature. NU-1000-CNF (3.5 mg, 1.5 μmol) was loaded into a 1.5 dram vial and 1 mL of 0.4 M *N*-ethylmorpholine solution (0.05 mL *N*-ethylmorpholine, 0.9 mL DI water/0.1 mL D_2O) was added and then stirred for 5 min to disperse homogeneously. 4 μL (25 μmol) of DMNP was

added to the mixture and swirled for 10 s. The reaction mixture was then transferred to an NMR tube and the NMR spectrum was immediately measured; the first data point was collected 120 s after the start of the reaction. The progress of the reaction was monitored in 1 min increments for 1 h (number of scans = 16, delay time = 28 s). The solvent was 10 % D_2O/H_2O.

Reusability test for hydrolysis with DMNP

To a 20 mL vial was added 3 mL of 0.15 M N-ethylmorpholine and 10 mg of NU-1000-CNF. The solution was sonicated for 1 minute and 12 μL of DMNP was added to the mixture. After 1 h, the mixture was centrifuged and the solvent was removed while the solid was washed with water and acetone in order to remove any product or un-reacted starting material from the MOF. Subsequently the solid residue was isolated using a filter and dried at 80^0C under vacuum for 12h. The hydrolysis reaction was then repeated as described above.

Preparation of NU-1000-CNF/cellulose composite and filter test

The MOF catalyst (10 mg) was dispersed in 10 mL of DI water, homogeneously. This suspension was filtered through a commercial cellulose filter (effective diameter: 25 mm) using vaccuum and then 10 μL of diethylchlorophosphate was passed though the MOF/cellulose composite.

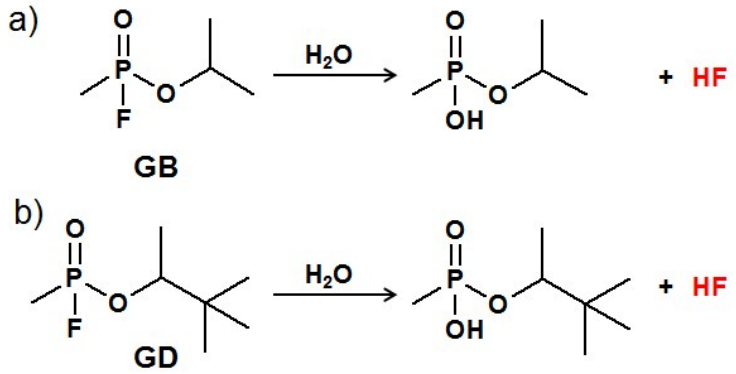

Figure S1. Hydrolysis reactions of nerve agents: a) *O*-Isopropyl methylphosphonofluoridate (GB) and b) *O*-Pinacolyl methylphosphonofluoridate (GD).

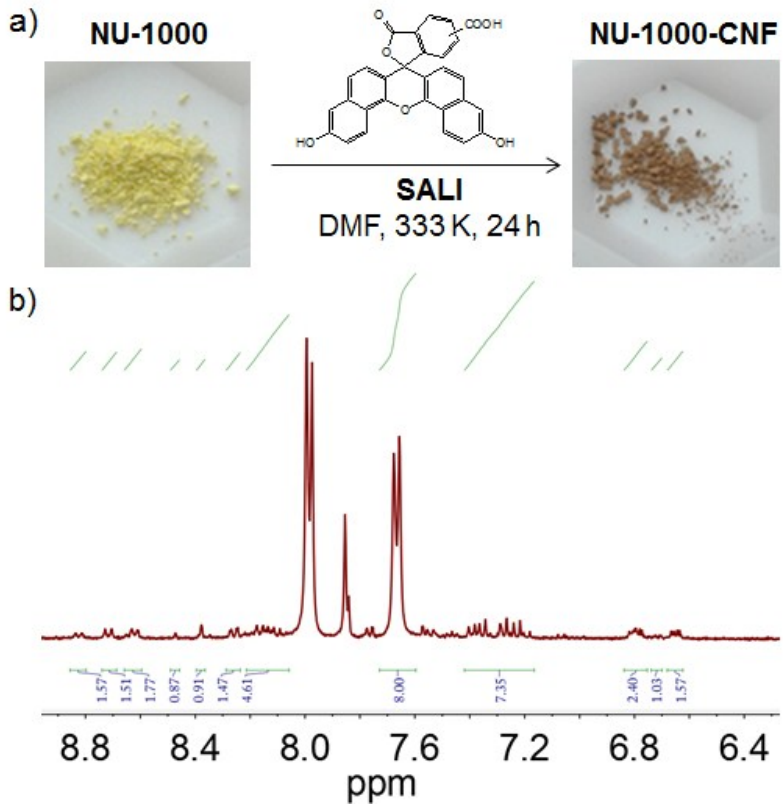

Figure S2. a) Colour change of NU-1000 after SALI and b) ^{1}H NMR spectrum of NU-1000-CNF in 10% D_2SO_4/DMSO

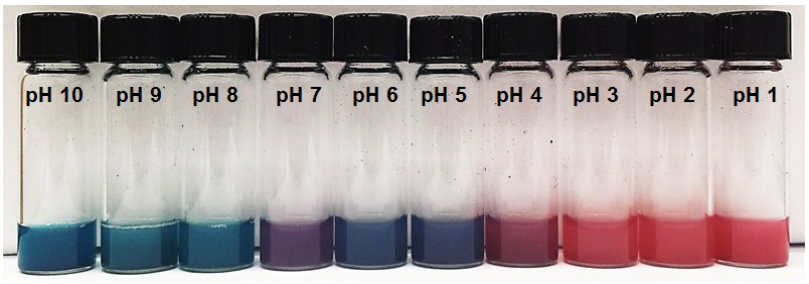

Figure S3. Colouration of NU-1000-CNF in various pH solution.

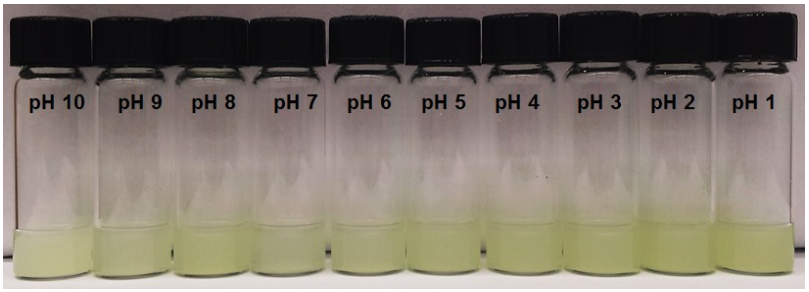

Figure S4. NU-1000 in various pH solution.

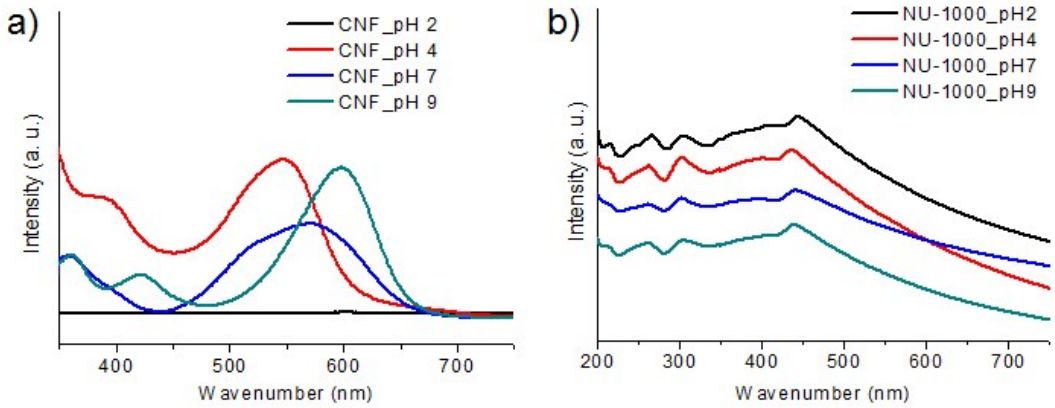

Figure S5. UV-vis absorption spectrum of a) 5(6)-carboxynaphthofluorescein and b) NU-1000 under various pH conditions.

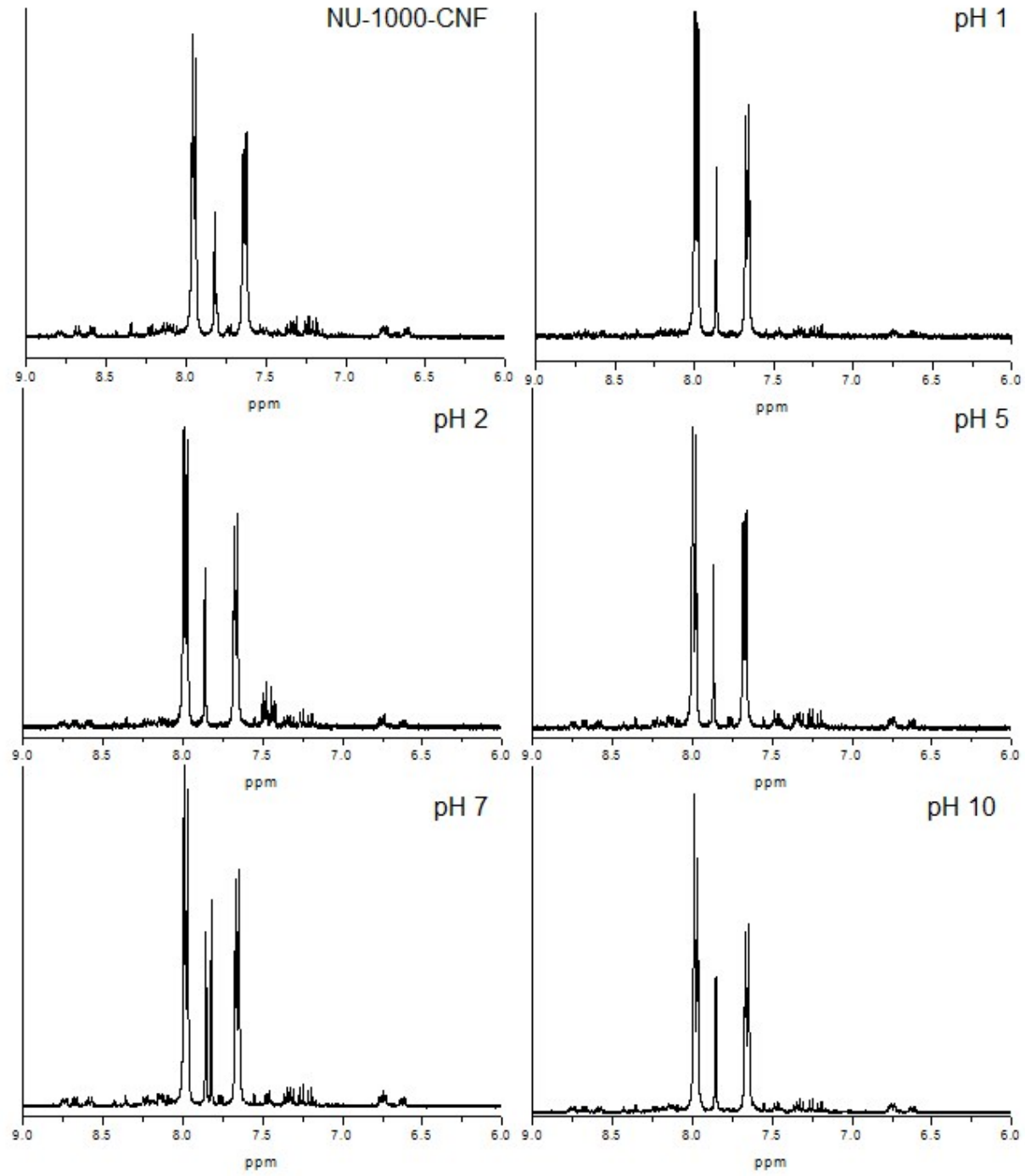

Figure S6. ^{1}H NMR spectra of NU-1000-CNF in 10% D_2SO_4/DMSO after soaking in the different pH solutions indicated.

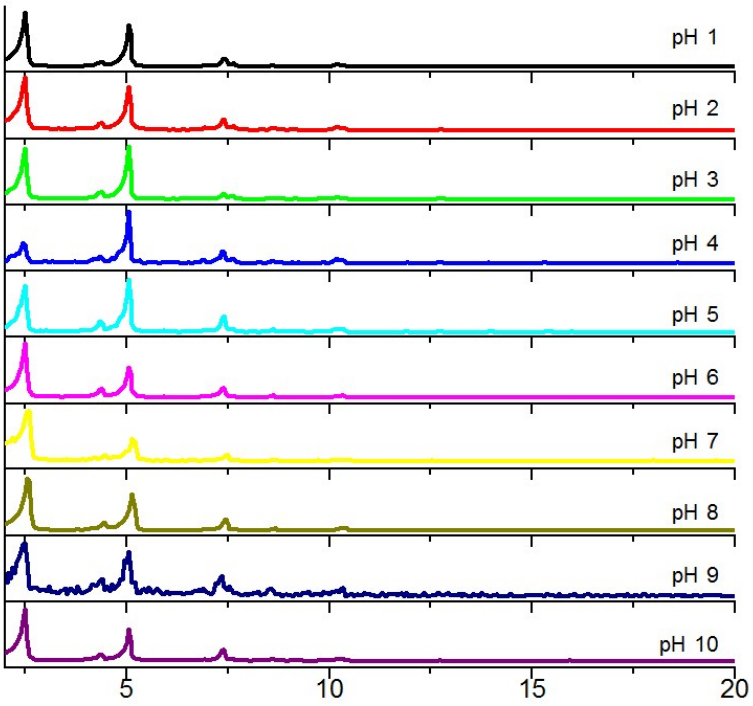

Figure S7. PXRD patterns for NU-1000-CNF after soaking in the different pH solutions indicated.

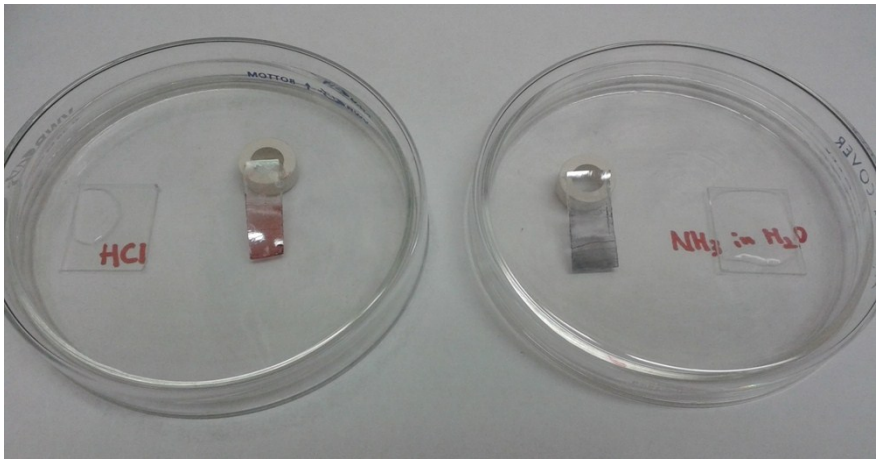

Figure S8. Thin films of NU-1000-CNF exposed to HCl and NH_3 vapour respectively. Samples were switched after washing with ethanol and the colour change is reversible (some of the MOF was detached from the substrate during washing because the interaction between NU-1000-CNF and glass is poor).

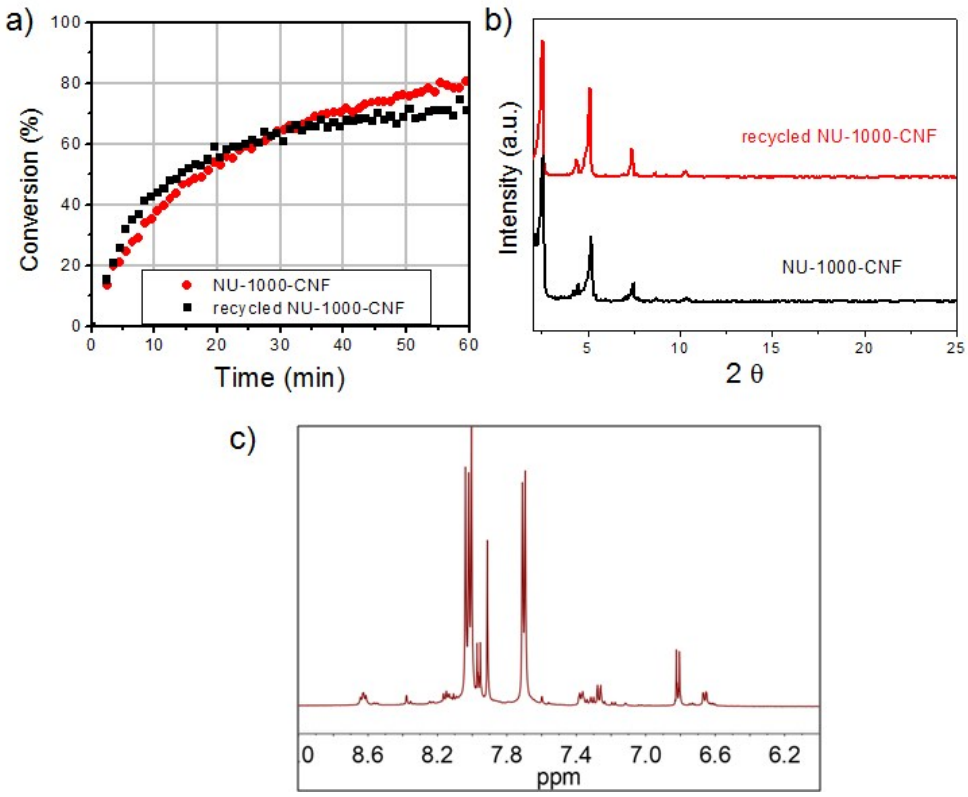

Figure S9. a) Catalytic hydrolysis of DMNP with NU-1000-CNF and recycled NU-1000-CNF and b) PXRD patterns of NU-1000-CNF before and after catalytic hydrolysis of DMNP c) ^{1}H NMR spectrum of NU-1000-CNF after catalytic hydrolysis of DMNP

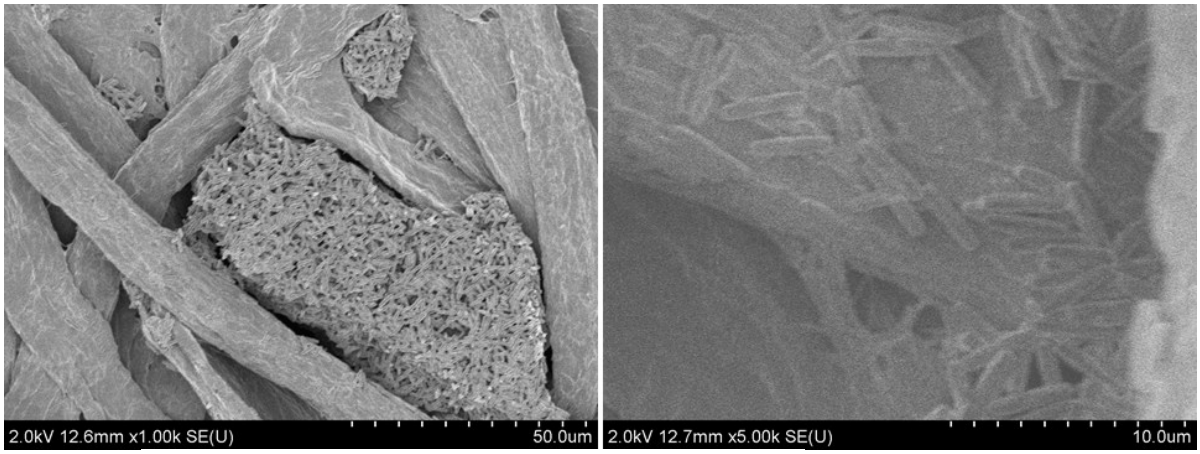

Figure S10. SEM images of NU-1000-CNF/cellulose composite

Reference

1. J. E. Mondloch, W. Bury, D. Fairen-Jimenez, S. Kwon, E. J. DeMarco, M. H. Weston, A. A. Sarjeant, S. T. Nguyen, P. C. Stair, R. Q. Snurr, O. K. Farha and J. T. Hupp, *J. Am. Chem. Soc.* 2013, ***135***, 10294.