<u>**Supporting Information**</u>

Non-isocyanate polyurethane (NIPU) Films for Dual-Function Humidity Sensing and Hydroplasticization Monitoring by harnessing Clusteroluminescence

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Contents

1.1. Materials

Trimethylol propane triglycidyl ether (TMPTE, Aldrich, technical grade); glycerol polyglycidylether (GTE, Thermo Fisher Scientific), 1,2-bis(2-aminoethoxy)ethane (EDR, TCI, >98%); 1,3-cyclohexanedimethanamine (BAC, TCI, >98%); hexamethylenediamine (HMDA, Alfa Aesar GmbH & Co KG, >98%), polyethyleneimine (PEI 25,000, branched, Aldrich, 99%, average M_n = 10,000 GPC); tetrabutylammonium iodide (TBAI, Aldrich, 99%); and potassium hydroxide (KOH, VWR, 90%) were used without further modification. Potassium hydroxide (>99.95, Sigma-Aldrich), potassium acetate (>99.0, Sigma-Aldrich), magnesium chloride (>98.0, VWR International), sodium iodide (>99.5, Sigma-Aldrich), magnesium nitrate (>99, Sigma-Aldrich), sodium bromide (>99, Sigma-Aldrich), potassium iodide (VWR International), sodium chloride (VWR International) and potassium chloride (99%, Acros Organics BVBA) were purchased and used for making humidity chambers.

1.2. Synthesis procedures

1.2.1. Trimethylolpropane tri-cyclic carbonate (TMPTC) synthesis

In a 250 mL high pressure reactor, trimethylolpropane triglycidyl ether (TMPTE, 60 g, 198.4 mmol) and tetrabutylammonium iodide (1830 mg, 2.73 mmol) were introduced. At 80 °C and 100 bar of CO_2, the cell was then brought to equilibrium. Under stirring, the reaction continued for 24 h. The product was then recovered upon depressurization, and any remaining CO_2 was eliminated under vacuum for 16 h at 60 °C. The full conversion of epoxide into five membered cyclic carbonate was checked by ^{1}H and ^{13}C NMR spectroscopy in $CDCl_3$ [1].

1.2.2. TMPTC synthesis in kilogram scale

In a 2.0 L high pressure cell reactor, 1.157 kg of TMPTE and 35.29 g of tetrabutylammonium iodide (TBAI, 2.5 mol% vs TMPTE) were added. Then the high-pressure cell was equilibrated at 110 °C for 24 h at constant pressure of 90 bar keeping stirring rate of 200 rpm. Finally, the stirring was stopped, and the cell was slowly depressurized at 110 °C. The as obtained viscous crude TMPTC of about 1,400 kg was obtained having yield of >98% as confirmed from the ^{1}H NMR in $CDCl_3$ [2]. Before introducing into formulation, product was degassed by thermal treatment at 80 °C for 16 h and then by vacuum treatment at 60 °C for 16 h.

1.2.3. Glycerol polyglycidyl carbonate (GTC) synthesis from Ipox CL 12 in kilogram scale

In a typical experiment, glycerol polyglycidylether (1 kg, GTE) was transferred into a 2 L cell high pressure reactor. Then, 35.48 g of tetrabutylammonium iodide (TBAI, 2.5 mol% vs GTE) were added prior closing the cell. The cell was then equilibrated at 110 °C for 24 h, keeping the CO_2 pressure constant to 90 bar and the stirring rate to 200 rpm. After reaction, the stirring was stopped and the cell slowly depressurized at 110 °C to maintain product as a very low viscous fluid. After removal of CO_2, the liquid product was collected (collected crude product > 1,250 kg) and analyzed by ^{1}H-NMR in $CDCl_3$, showing a yield of > 98%.[2] Before use, product was degassed by thermal treatment at 80 °C for 16 h and then by vacuum treatment at 60 °C for 16 h.

Reference

[1] M. Bourguignon, B. Grignard, C. Detrembleur, *Angew Chem Int Ed* **2022**, *61*, e202213422.
[2] M. Bourguignon, B. Grignard, C. Detrembleur, *J. Am. Chem. Soc.* **2024**, *146*, 988.

1.2.4. Synthesis of polyethyleneimine functionalized NIPU foam with EDR amine

TMPTC (5 g, 5CC = 34.5 mmol) and polyethyleneimine (200 mg) were added in a 4 × 4 cm^2 silicon mold and were mixed at room temperature (~20 °C) for 5 min to get a homogeneous viscous mixture. Then, water (600 mg, 33.33 mmol), EDR (1910 mg, NH_2 = 25.78 mmol) and KOH (90 mg, 1.38 mmol) were added to the formulation, and the formulation was mixed well for another 1 min to obtain homogeneous mixture. Then the formulation (homogeneous mixture) was positioned in a preheated oven at 100 °C for 4 h.

1.2.5. Synthesis of non-foamed NIPU

TMPTC (5 g, 5CC = 34.5 mmol) and polyethyleneimine (200 mg) were added in a 4 × 4 cm^2 silicon mold and were mixed at room temperature (~20 °C) for 5 min to get a homogeneous viscous mixture. Then, EDR (1910 mg, NH_2 = 25.78 mmol) and KOH (90 mg, 1.38 mmol) were added to the formulation, and the formulation was mixed well for another 1 min to obtain homogeneous mixture. Then the formulation (homogeneous mixture) was positioned in a preheated oven at 100 °C for 4 h.

1.2.6. Synthesis of polyethyleneimine functionalized NIPU foam with BAC amine

Foam containing 1,3-cyclohexanedimethanamine was synthesized according to the following procedure: TMPTC (5 g, 5CC = 34.7 mmol), polyethyleneimine (200 mg), water (300 mg, 16.67 mmol), BAC (1850 mg, NH_2 = 26.00 mmol) and KOH (90 mg, 1.60 mmol) were added thoroughly in a 4 × 4 cm^2 silicon mold and were mixed for 1 min at room temperature (~20 °C) to create a homogeneous mixture. After that the homogeneous mixture was placed in a pre-heated oven at 80 °C for 5 h. The foam was demolded after cooling to room temperature and finally stored at room temperature under ambient condition.

1.2.7. Synthesis hybrid petro-based NIPU foam with EDR at room temperature by cascade exotherms

The room temperature NIPU foam was prepared following the following process: Initially glycerol polyglycidyl carbonate (TMPTC, 17.9 g, 5CC = 124 mmol), TMPTE (12.5 g, epoxide = 124 mmol), hydrotalcite (4.30 g, 24 wt.%) were mixed together in a plastic vial until the mixture was homogeneous. In a second vial, EDR (11.20 g, NH2 = 151 mmol) and TREN (3.17 g, NH2 = 65 mmol) were mixed together at room temperature. Then, the mixed amines solution was added into the TMPTC/TMPTE mixture. Rapidly, KOH (0.84 g, 15 mmol) solubilized in water (0.56 g, 31 mmol) was added to initiate foaming.

1.2.8. Synthesis of hybrid bio-based NIPU foam with HMDA at room temperature by cascade exotherms

The **90% bio-based foam** was prepared following the following process: Initially glycerol polyglycidyl carbonate (GTC, 22.6 g, 5CC = 172 mmol), glycerol polyglycidylether (GTE, 7.49 g, epoxide = 86 mmol), Cloisite Na (3 g) were mixed together in a plastic vial until the mixture was homogeneous. In a second vial, HMDA (8.76 g, NH2 = 151 mmol) and TREN (3.12 g, NH2 = 65 mmol) were mixed together at 40 °C to melt HMDA. Then, the amine solution was left for cooling to 30 °C (till the first trace of recrystallization appears) and added into the GTP/GTE mixture with parallel increase of the formulation temperature. Rapidly, KOH (1.14 g, 21.6 mmol) solubilized in water (0.78 g, 43 mmol) was added to initiate foaming.

1.3. Recycling procedures

1.3.1. Recycling of polyethyleneimine functionalized NIPU foam with EDR to film

Recycling of polyethyleneimine functionalized NIPU foams were performed in Press Data Plate-CARVER (Model: 4122CE4010C00, serial NO.: 190142). Foams of 2.3 cm of thickness were introduced into the various preheated hot-press for different time interval as mentioned in the Table S1. At first the polyethyleneimine functionalized NIPU foam was pressed by the constant said pressure and initially the pressure was released three time for 5 mins of interval to avoid cracks in the film.

Table S1: Preparation of three different NIPU films by changing the reprocessing conditions

Film	Pressure (Ton)	Temperature (°C)	Time (h)
Film-a	1	160	2
Film-b	2	170	3
Film-c	2	170	5

The film-a is not crack free, however, film-b and film-c are crack free and smooth for further characterization and humidity sensing application.

1.3.2. Recycling of polyethyleneimine functionalized NIPU foam with BAC to film

Recycling of polyethyleneimine functionalized NIPU foam with BAC amine was performed in Press Data Plate-CARVER (Model: 4122CE4010C00, serial NO.: 190142). Foams of about 2.5 cm of thickness were introduced into the hot-press at 170 °C for 3 h. At first the foam was pressed by the constant pressure of 2 ton and initially the pressure was released three time for 5 mins of interval to avoid cracks in the film.

1.3.3. Recycling of room temperature NIPU foam to film

Recycling of room temperature NIPU foam with EDR amine was performed in Press Data Plate-CARVER (Model: 4122CE4010C00, serial NO.: 190142). Foams of about 2.7 cm of thickness were introduced into the hot-press at 170 °C for 3 h. At first the foam was pressed by the constant pressure of 2 ton and initially the pressure was released three time for 5 mins of interval to avoid cracks in the film.

1.3.4. Recycling of hybrid bio-based NIPU foam with HMDA to film

Recycling of hybrid bio-based NIPU foam with HMDA amine was performed in Press Data Plate-CARVER (Model: 4122CE4010C00, serial NO.: 190142). Foams of about 2.5 cm of thickness were introduced into the hot-press at 170 °C for 3 h. The foam was pressed by the constant pressure of 2 ton and initially the pressure was released three time for 5 mins of interval to avoid cracks in the film.

1.4. Characterization techniques

1.4.1. ATR-Infrared analysis

Attenuated transmission reflectance (ATR) Infrared (IR) spectra were recorded by a Nicolet IS5 spectrometer (Thermo Fisher Scientific) equipped with a transmission or with a diamond ATR device. Spectra were obtained in transmission or ATR mode as a result of 32 spectra in the range of 4000-500 cm^{-1} with a nominal resolution of 4 cm^{-1}. Spectra were further processed by the OriginPro 9.0 software.

1.4.2. Thermogravimetric analysis (TGA)

TGA analysis was performed on a TGA2 instrument from Mettler Toledo. Around ~8 mg of sample was flushed with nitrogen (20 mL min^{-1}) for 10 min at 25 °C. The sample was then heated at 10 °C min^{-1} until 600 °C under a nitrogen atmosphere (20 mL min^{-1}).

1.4.3. Dynamic scanning calorimetry (DSC)

DSC study was performed on a DSC Q2000 differential calorimeter (TA Instruments). All the experiments were performed under ultrapure nitrogen flow. We used only one heating cycle for the T_g measurements to avoid any aging/evolution of the sample during multiple heating cycles. Samples of ~5 mg were used and placed in sealed aluminum pans. The samples were first cooled down to −80 °C at a rate of 10 °C min^{-1} and then heated to 100 °C at 10 °C min^{-1}.

1.4.4. Scanning electron microscopy (SEM)

Scanning electron microscopy (SEM) was recorded with a QUANTA 600 apparatus microscope from FEI with a piece of foam dried in a desiccator.

1.4.5. Tensile test

Tensile tests were performed on an INSTRON (model 34TM-10) device integrated with Aide Bluehill Universal software. The elongation was performed at a rate of 5 mm min^{-1} on dog bone samples of ~length = 15 mm, ~width = 5 mm and ~thickness = 0.3 mm. Tensile modulus was calculated by the slope at the beginning (i.e. 2-5 strain %) of the stress-strain curve. The experiment was performed with three replicates.

1.4.6. Fluorescence spectroscopy

Fluorescence full scan spectra of photoluminescent foams/ films and water absorbed foams/ films were recorded within 350–800 nm using the spectrofluorometer (Tecan Infinite 200Pro) using 350–520 nm of excitation wavelengths (λ_{ex}s). UV-star® microplate, 96 well, half area, µclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence spectra were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 µs, 0 µs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively.

1.4.7. Fluorescence lifetime imaging (FLIM) study

Fluorescence lifetime images of the NIPU foams/ films were recorded with the Leica Stellaris 8 confocal microscope (Leica Microsystems, Wetzlar, Germany) equipped with a pulsed white laser of 440 nm as the excitation source, and hybrid power detectors. Raw images were recorded (1024 x 1024 format) by scanning an area of 581.25 µm x 581.25 µm. A Leica HC PL APO 20x/0.70 dry objective was used. Regarding the acquisition parameters, a zoom factor of 1 and an optical section of 0.896 µm were fixed, performing 10 frame repetitions for each measurement. The frame rate was 0.389 s^{-1} and the pixel dwell time was 512 ns. To analyse FLIM results, the Fiji software (FLIMJ and TRI2) was used. The phasor analysis system analyses fluorochrome lifetime data according to a point cloud of space vectors in a semicircle. This vector space will position each image pixel according to its lifetime within this semicircle. A consistent scale of 2–4 ns was used.

1.4.8. Fluorescence microscopic imaging

The fluorescence imaging of the foams was carried out by Confocal Zeiss LSM 880. The images were analyzed using the advanced PicoQuanta software. The laser sources of 454, 488, 514, 543, 594 and 633 nm were used for the measurements.

1.5. Methodology

1.5.1. Swelling experiments of the NIPU foam/ film

Foam/ film was dried in an over at 50 °C for 2 h or in desiccator for 24 h. The initial mass (m_i) of the dried NIPU foam/ film was measured. Then, swelling of the foam/ film was performed by immersing of the dried foam/ film in THF for 24 h. After 24 h, swollen foam was weighted and mass (m_t) were recorded. The swelling of the NIPU foam/ film after 24 h was measured by the formula:

$$\text{Swelling (\%)} = (m_t - m_i)/m_i \times 100$$

1.5.2. Gel content

As synthesized NIPU foam/ film was cut into small portions and initial mass (m_1) was taken. Then, the foam/ film was dissolved in in THF for 24 h. After that, THF was removed and foam/ film was dried at room temperature and under vacuum at 60 °C for 48 h and 16 h, respectively, and final mass (m_2) was taken. Finally, gel content (GC) was calculated by the formula:

$$GC = (m_2/m_1) \times 100$$

1.5.3. Preparation of humidity chambers

The humidity chambers of specific humidity were prepared by saturated salt solution in water (Table S3) and put them in a hermetically sealed containers following the procedure at literature.[1] Few pieces of films/ foams samples were placed in the chamber for 24 h for equilibrium and then further use for different tests.

1.5.4. Water content measurement

After hot pressing at 170 °C, all NIPU films were stored in a desiccator or subjected to vacuum drying to eliminate residual moisture. The films were then equilibrated in humidity chambers maintained at relative humidity (RH) levels ranging from 10% to 85%. Following equilibration, the samples were removed and subjected to thermogravimetric analysis (TGA) in the temperature range of 30–200 °C. The water content (%) was determined from the mass loss at 170 °C, as obtained from the TGA profiles.

1.5.5. The fluorescence reversibility test

The reversibility of the fluorescence response of the NIPU film-b under varying humidity conditions was evaluated using a controlled humidity cycling protocol. Initially, pieces of NIPU film-b were placed in a humidity chamber maintained at 40% RH, 60% RH and 80% RH, and allowed to equilibrate for 24 h for each RH level. Fluorescence measurements were then conducted at 520 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 450 nm of excitation wavelength (λ_{ex}), enabling precise monitoring of intensity changes at each RH level. For checking reversibility, the NIPU pieces initially equilibrated at 80% RH for 24h was transferred to lower humidity environments (40% RH and 60% RH) and maintained for an additional 24 h to ensure complete equilibration at each condition. Fluorescence spectra were then recorded under similar conditions and compared to initial humidity-induced fluorescence response. Results are shown in Figure S18c.

1.5.6. Graphics based analyses

All graphics-based analyses were carried out by Origin 9.0, ChemDraw Ultra 12.0, Gaussian 16, GaussSum 6.0, Multiwfn_3.8, IrfanView 64, VMD1.9.4a53 and design expert 7.0 softwares.

Table S2: Excitation-dependent emission properties of all NIPU films showing CIE coordinates (Figures are included in the Figure 3d-f)

Wavelength (nm)	**NIPU film-a**		**NIPU film-b**		**NIPU film-c**	
	x	y	x	y	x	y
330 nm	0.19918	0.21613	0.21519	0.23804	0.24177	0.26969
350 nm	0.19218	0.20776	0.20556	0.22603	0.23556	0.26258
360 nm	0.19179	0.21243	0.20428	0.22749	0.23444	0.26421
370 nm	0.19331	0.22243	0.20480	0.23530	0.23596	0.27249
380 nm	0.19611	0.23530	0.20872	0.24829	0.23848	0.28132
390 nm	0.19976	0.25086	0.21441	0.26679	0.24178	0.29237
400 nm	0.20465	0.27553	0.22205	0.29399	0.24785	0.31247
410 nm	0.21518	0.32357	0.23616	0.34162	0.26120	0.35267
420 nm	0.23295	0.39127	0.25825	0.40783	0.28342	0.41054
430 nm	0.25420	0.45885	0.28284	0.47127	0.30804	0.46663
440 nm	0.28062	0.52432	0.31157	0.52824	0.33582	0.51818
450 nm	0.30948	0.57199	0.34017	0.56495	0.36299	0.55183
460 nm	0.33840	0.59559	0.36558	0.58069	0.38656	0.56516
470 nm	0.36817	0.59708	0.38975	0.58046	0.40799	0.56519
480 nm	0.39821	0.58426	0.41614	0.5684	0.43128	0.55462
490 nm	0.42776	0.56324	0.44289	0.54898	0.45558	0.53693
500 nm	0.45944	0.53593	0.47264	0.52312	0.48159	0.51443
520 nm	0.52835	0.47043	0.53945	0.45942	0.54144	0.45744

2. Humidity sensing by NIPU foam

Fluorescence measurement for humidity sensing study

The fluorescence of water absorbed foams taking from different humidity chambers (10-85%) were recorded at 490 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 420 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, µclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 µs, 0 µs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced foam. All the results were done twice with three replicates.

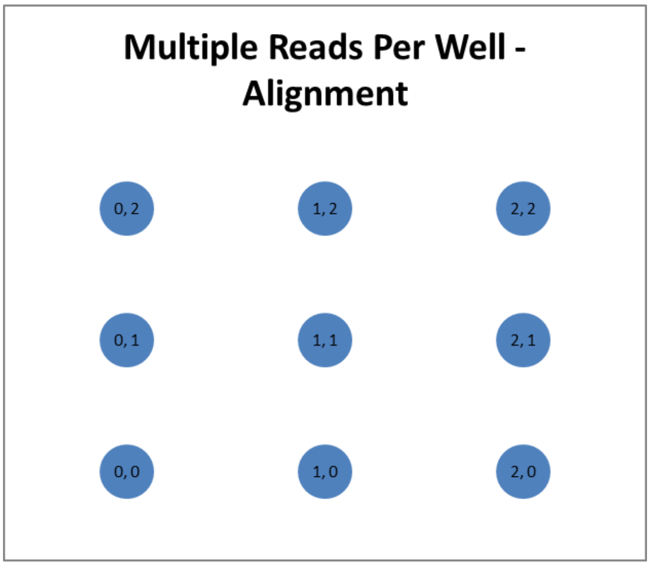


Table S3: Selected Saturated Salt Solution for Creating Humidity[1]

Salt used	**Relative humidity at 15 °C**	**Relative humidity at 20 °C**	**Relative humidity at 25 °C**
Potassium hydroxide	10.68 ± 1.10	9.32 ± 0.90	8.23 ± 0.72
Potassium acetate	23.40 ± 0.32	23.11 ± 0.25	22.51 ± 0.32
Magnesium chloride	33.30 ± 0.21	33.07 ± 0.18	32. 78 ± 0.16
Sodium iodide	40.88 ± 0.70	39.65 ± 0.59	38.17 ± 0.50
Magnesium nitrate	55.87 ± 0.27	54.38 ± 0.23	52.89 ± 0.22
Sodium bromide	60.68 ± 0.51	59.14 ± 0.44	57.057 ± 0.40
Potassium iodide	70.98 ± 0.28	69.90 ± 0.26	68.86 ± 0.24
Sodium chloride	75.6 1 ± 0.18	75.47 ± 0.14	75.29 ± 0.12
Potassium bromide	82.62 ± 0.22	81.67 ± 0.21	80.89 ± 0.21
Potassium chloride	85.92± 0.33	85.11± 0.29	84.34± 0.26

References:

[1] Lewis Greenspan, Journal of Research of the National Bureau of Standards- A. Physics and Chemistry, 1977, 81 A, (1), 89-96.

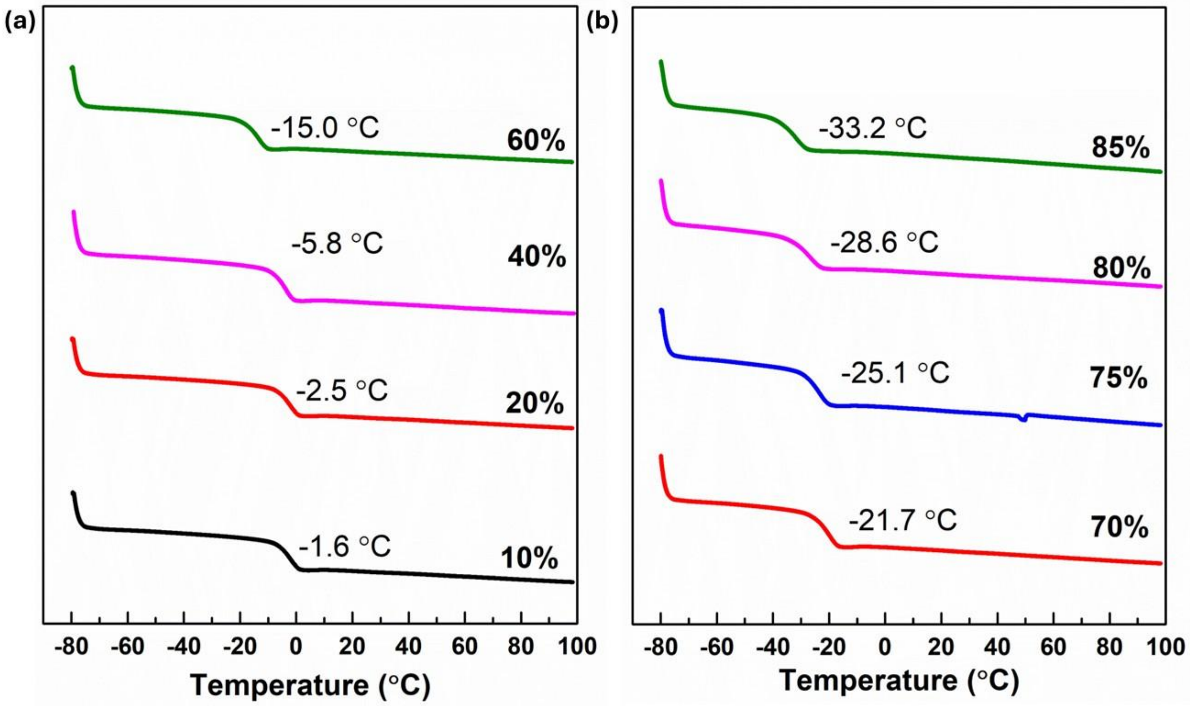


Figure S1. DSC thermograms of NIPU foam at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

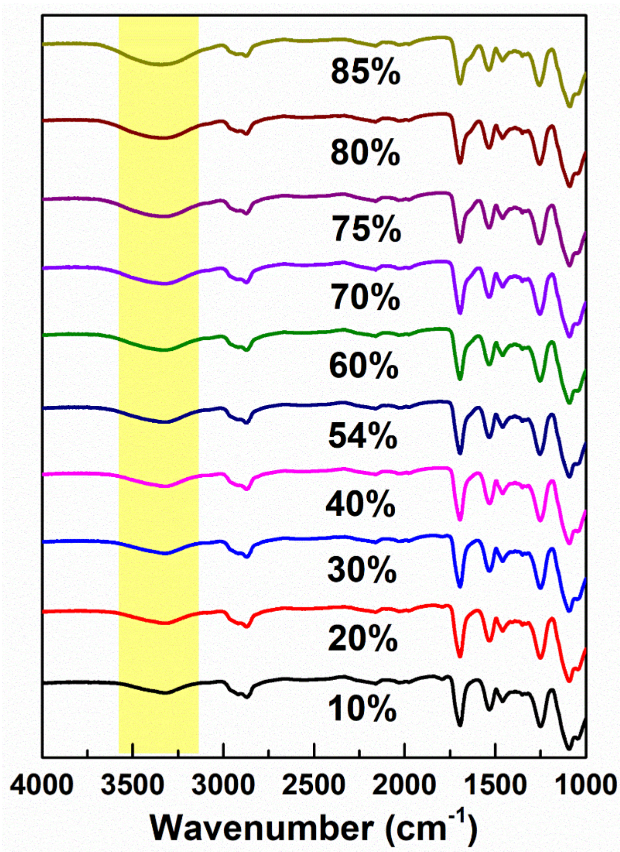


Figure S2. ATR-infrared spectra of NIPU foams at different humidities (10%, 20%, 30%, 40%, 54%, 60%, 70%, 75%, 80% and 85%)

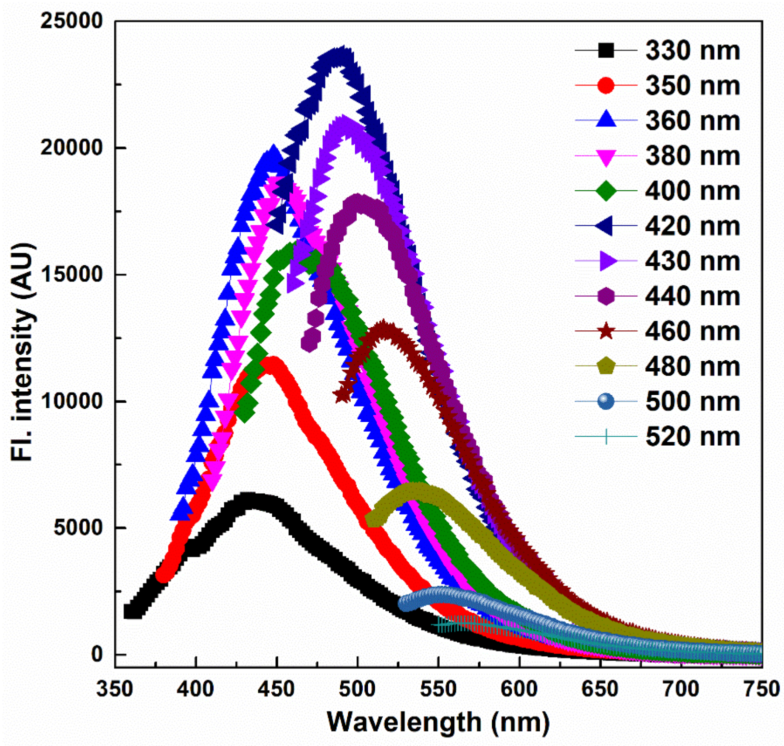


Figure S3. Fluorescence spectra of NIPU foam using excitation wavelength (λ_{ex}) = 300-520 nm

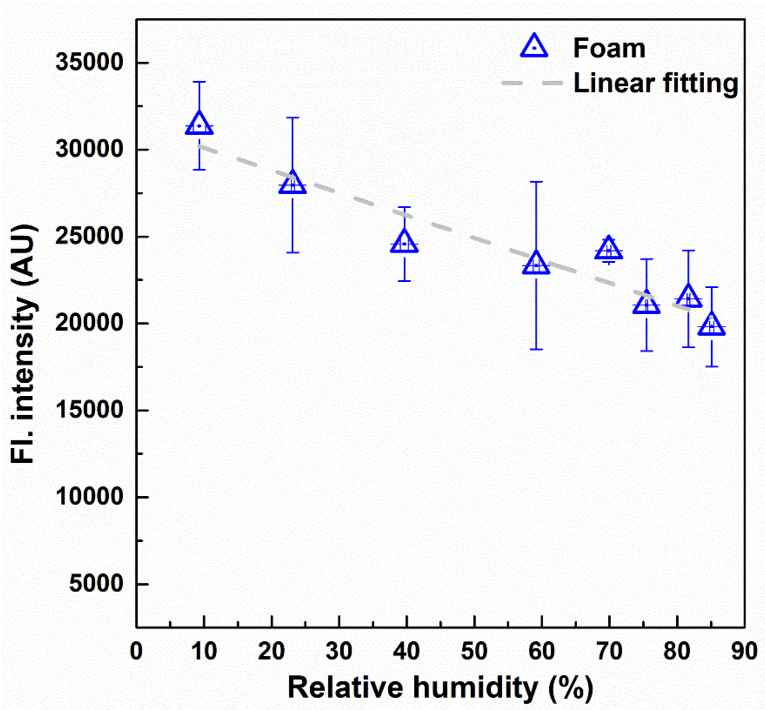


Figure S4. The change in fluorescence intensity of NIPU foam with relative humidities (10-85%)

3. Calibration data analysis and figures of merit

In this study, each sensor was calibrated by measuring the analytical signal, that is the fluorescence intensity (FI, y_i), at eight different relative humidity (RH, x_i) levels, with three replicate measurements per level. Due to the limited number of replicates (3 for each RH level), statistical tests for normality and homoscedasticity within each RH level lack robustness. Therefore, calibration curves were constructed using the mean signal at each RH level, which improves data stability and enhances the likelihood that residuals follow a normal distribution.

The calibration curve was obtained using ordinary least squares linear regression, providing the following figures of merit as recommended in literature [1]: - Calibration sensitivity (slope, noted m) - Standard error of the slope (S_m) - intercept (noted b) – Standard error of the intercept (S_b) - Adjusted coefficient of determination (Adjusted R^2) – Standard error of the fit (S_y)

Standard error of the fit was calculated as follows:

$$S_y = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

where y_i is the observed mean signal at RH level i, $\hat{y}_i$ is the predicted signal from the linear model (m*x_i-intercept), and n is the number of RH levels. S_y estimates the standard deviation of the of the sensor response.

$$S_m = S_y\sqrt{\frac{n}{D}};\ S_b = S_y\sqrt{\frac{\sum_{i=1}^{n}(x_i)^2}{D}}\ with\ D = n\sum_{i=1}^{n}(x_i)^2 - (\sum_{i=1}^{n}(x_i)^2$$

Analytical sensitivity (γ)

Analytical sensitivity was calculated according to the definition by Mendel and Stiehler, which incorporates both the slope of the calibration and the measurement precision [2]:

$$\gamma = \frac{|m|}{\sigma_s};\ in\ this\ work = \frac{|m|}{S_y}$$

where m is the slope of the calibration curve and σ_s is the standard deviation of the analytical signal measurement. In this work, σ_s was taken as the standard error of the fit (S_y)

The relative humidity at the limit of detection (X_{LOD})

The relative humidity at the limit of detection was computed using the conventional formula:

$$X_{LOD} = \frac{t * \sigma_s}{|m|}; in\ this\ work = \frac{t * S_y}{|m|}$$

where t is the Student's t-value one tailed corresponding to 99% confidence and n − 2 degrees of freedom (in our case t = 3.143), σ_s is usually corresponding to the standard error of the signal, which is obtained by averaging the signal near the LOD [3]. In this work, σ_s was chosen as the standard error of the fit. σ_s is sometimes chosen as the standard deviation of the blank [3], which is not realistic in our case. First the blank corresponding to a RH of 0 % (dried sample) is not in the linear range and its variability (standard deviation) is very low compared to the variability at the tested RH (10-85 %).

References:

[1] DeMello, A. J. I'm Sensitive about Sensitivity. *ACS Sens.* **2022**, *7*, 1235–1236. https://doi.org/10.1021/acssensors.2c00982.

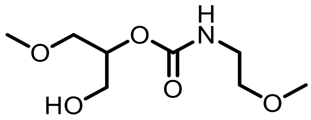
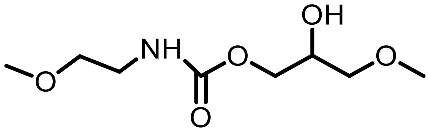
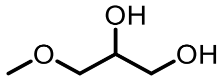
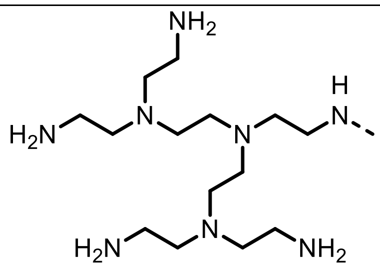
[2] Mandel, J.; Stiehler, R. D. Sensitivity-A Criterion for the Comparison of Methods of Test. *J. Res. Natl. Bur. Stand.* **1954**, *53*, 155–159.

[3] Loock, H.-P.; Wentzell, P. D. Detection limits of chemical sensors: Applications and misapplications, *Sens. Actuators B Chem.* **2012**, 173, 157–163. https://doi.org/10.1016/j.snb.2012.06.071.

Table S4: Summary table with the slope (m), standard error of the slope (S_m), intercept (b), standard error of the intercept (S_b), adjusted R^2, standard error of the fit (S_y), analytical sensitivity (AS), and the relative humidity at the limit of detection (X_{LOD}) for each sensor.

Sensors	Calibr. Sensit. (slope, m)	std error slope (S_m)	Intercept (b)	std error intercept (S_b)	Adj R^2	Std error fit (S_y)	RH_{LOD}	Analytical sensitivity (γ)	F.I. Blank (AU)	Std. dev blank
foam	-130	16.3	31396	1004	0.899	1224	30	0.106	33555	29
film-a	-84	5.9	12627	364	0.966	443	17	0.189	11724	11
film-b	-102	2.0	19690	123	0.997	150	5	0.680	19653	12
film-c	-90	3.0	18498	187	0.992	228	8	0.396	18540	13
Hybrid petro-based NIPU film	-55	1.5	14774	95	0.995	115	7	0.478	15403	18
Hybrid bio-based NIPU film	-113	4.6	21946	281	0.989	343	10	0.330	22634	20
BAC-based NIPU film	na	na	na	na	na	na	na	na	17851	27

4. Computational study to explain the multicolor emission

Structures of the model compounds used to make the aggregates		
 **Model compound-1**	 **Model compound-2**	 **Model compound-3**
 **PEI**		

Protocols for optimization and energy levels extraction

To make the analysis more convenient, molecules were fragmented to model compounds. For our system, the functionalized NIPU backbones were represented by model compound-1, model compound-2 and model compound-3, which are the main component of the molecules. All best possible configurations of each model compound were optimized in the ground state with Gaussian 16 (Consortium des Équipements de Calcul Intensif: CÉCI clusters) by density functional theory (DFT) using B3LYP functional and 6-311G basis set with default spin, zero charge and singlet spin. Subsequently, the lowest energy configuration was screened [1]. To investigate the mechanism of multicolor fluorescence and explore the inter chain interactions between chains, model NIPU film were created by making a small aggregation of model compounds: “1+2+3+PEI”. Moreover, moderate (2×(1a+2a+3+PEI)) and large (3×(1a +2a+3+PEI)) aggregates were constructed from the model compounds. All the aggregates were computed theoretically via density functional theory (DFT) using B3LYP functional and 6-311G basis set with default spin, zero charge and singlet spin. All the optimized structures showed non-imaginary frequencies. The energy levels of HOMOs/ LUMOs were calculated using GaussSum2.2. The orbitals were extracted using GaussView6.0.16.

Reference:

[1] M. Mahapatra, M. Bourguignon, B. Grignard, M. Vandevenne, M. Galleni, C. Detrembleur, Angew. Chem. Int. Ed. 2024, https://doi.org/10.1002/ange.202413605.

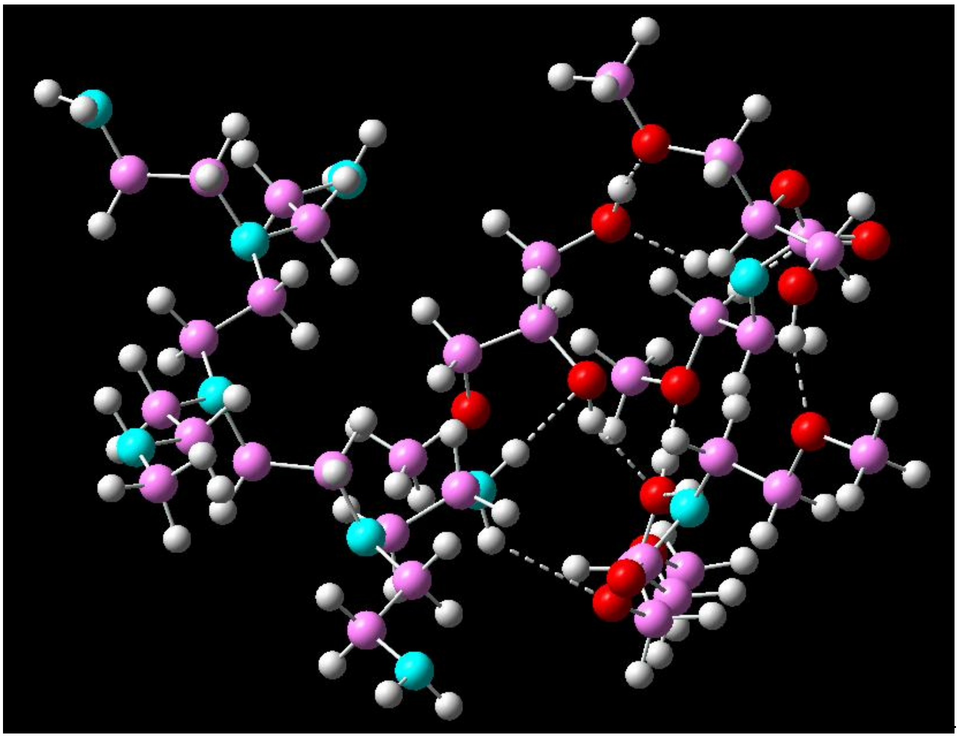


Figure S5. Optimized structure of aggregate (1+2+3+PEI) representing the NIPU film showing intra molecular hydrogen bonding interactions

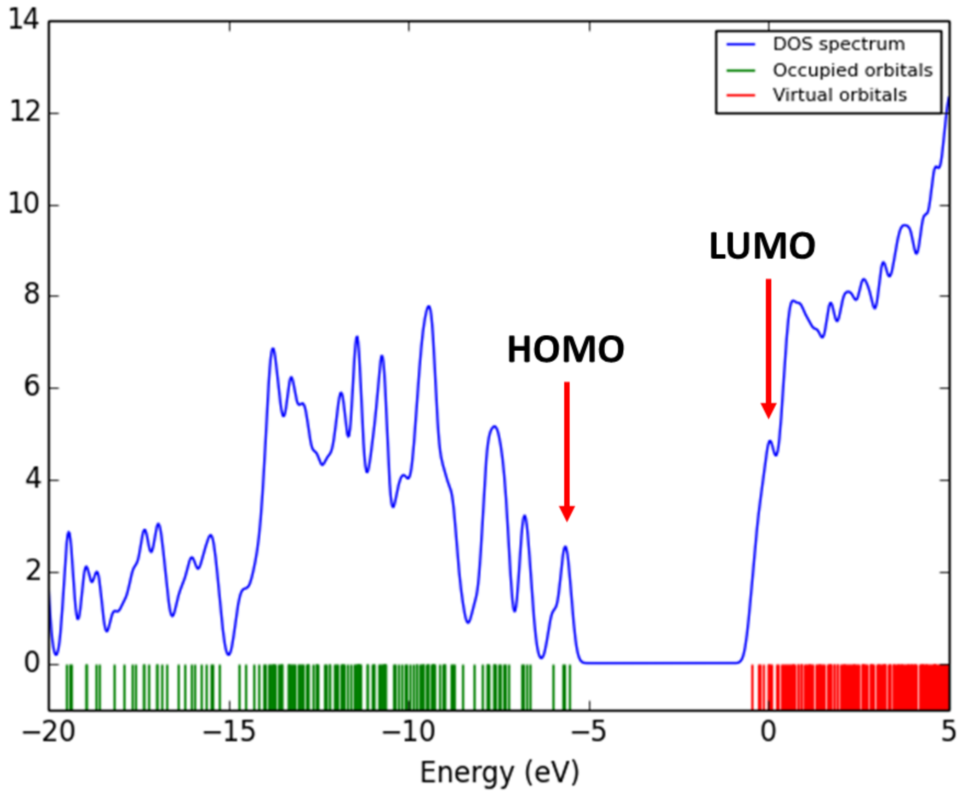


Figure S6. Density of state spectrum of small aggregate (1+2+3+PEI) representing the NIPU film using B3LYP/6-311 level in the range of -20 to 5 eV

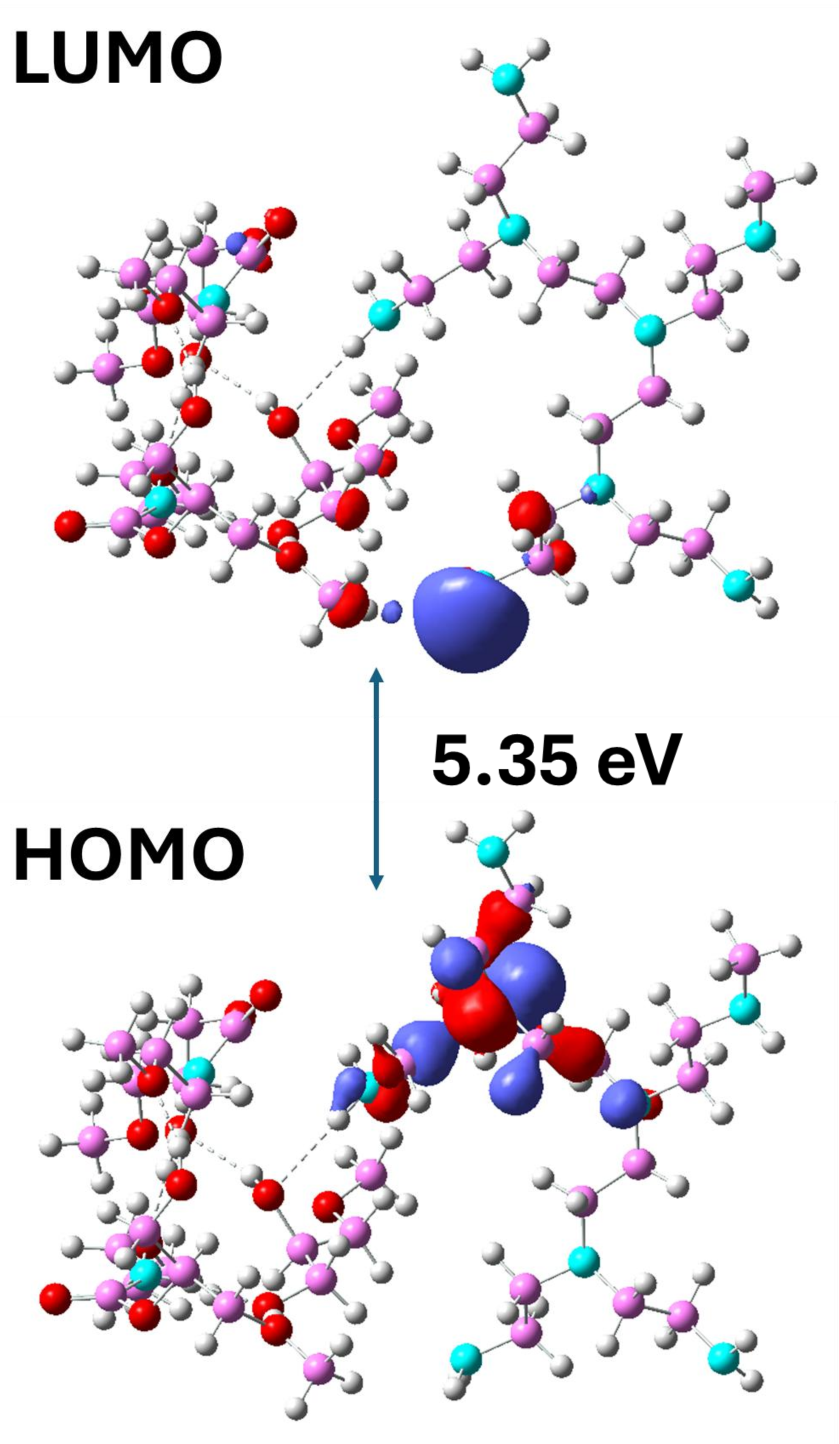


Figure S7. HOMO and LUMO of small aggregate (1+2+3+PEI)

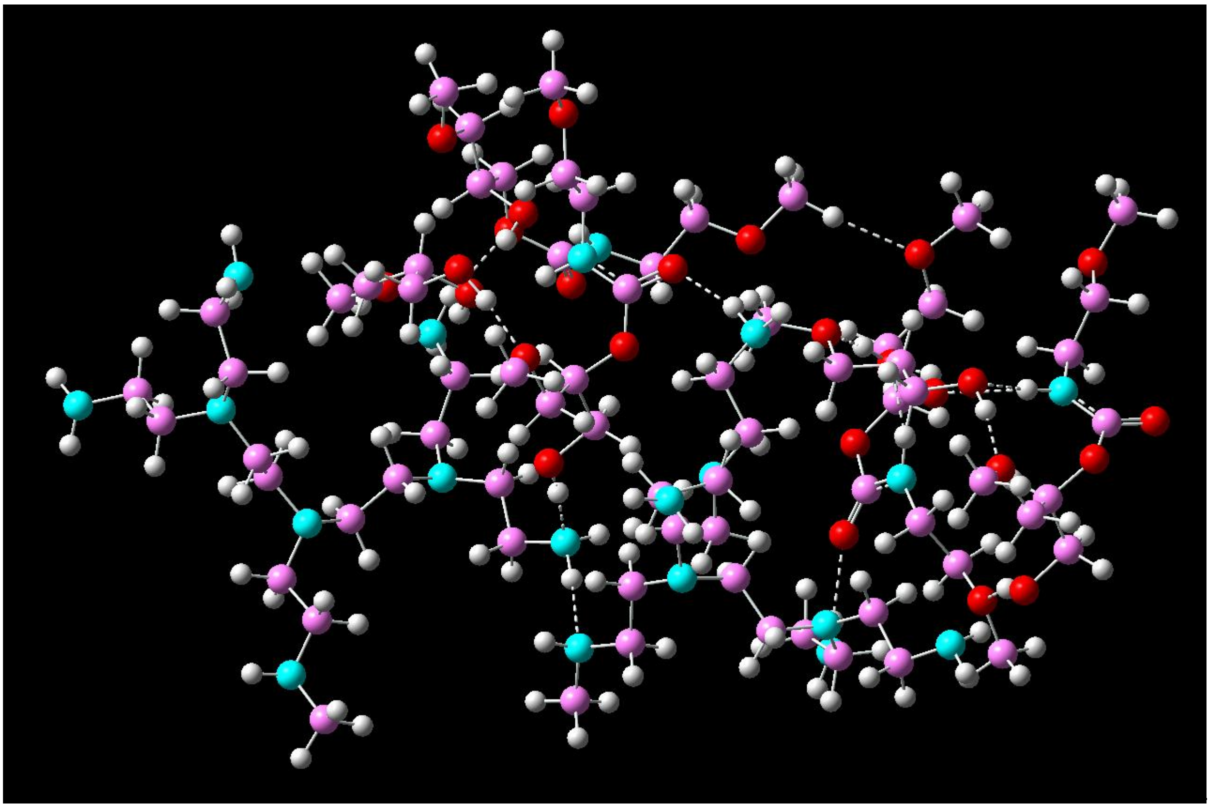


Figure S8. Optimized structure of moderate aggregate (2 x (1+2+3+PEI)) showing intra molecular hydrogen bonding interactions

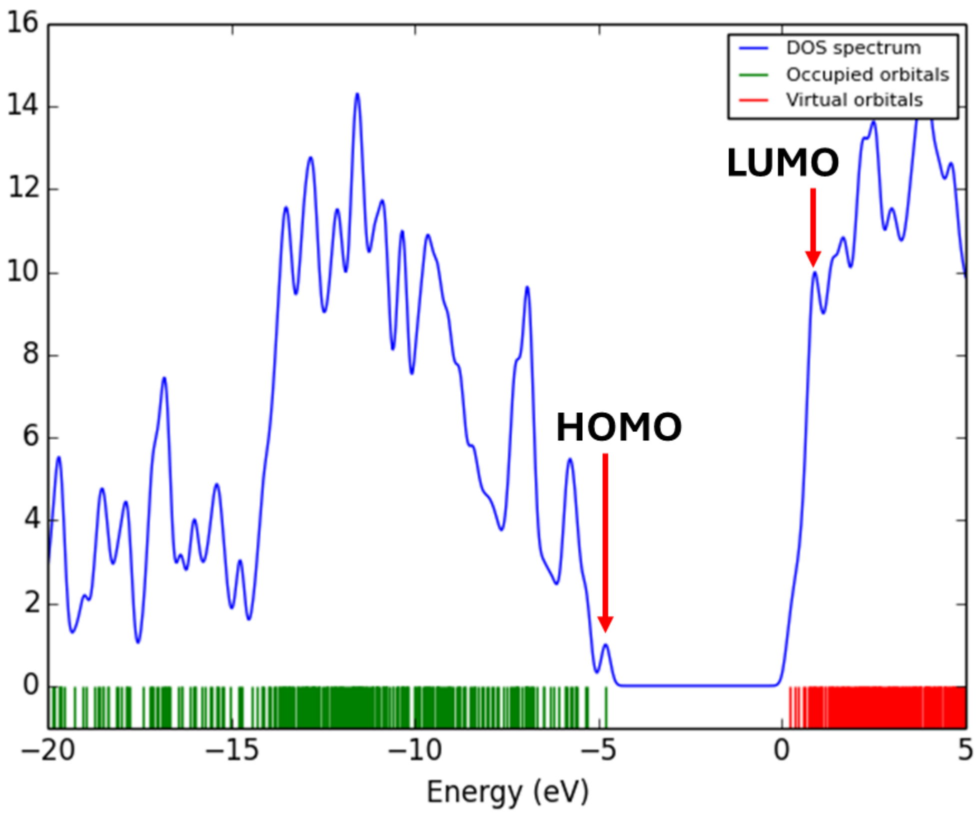


Figure S9. Density of state spectrum of moderate aggregate (2 x (1+2+3+PEI)) using B3LYP/6-311 level in the range of -20 to 5 eV

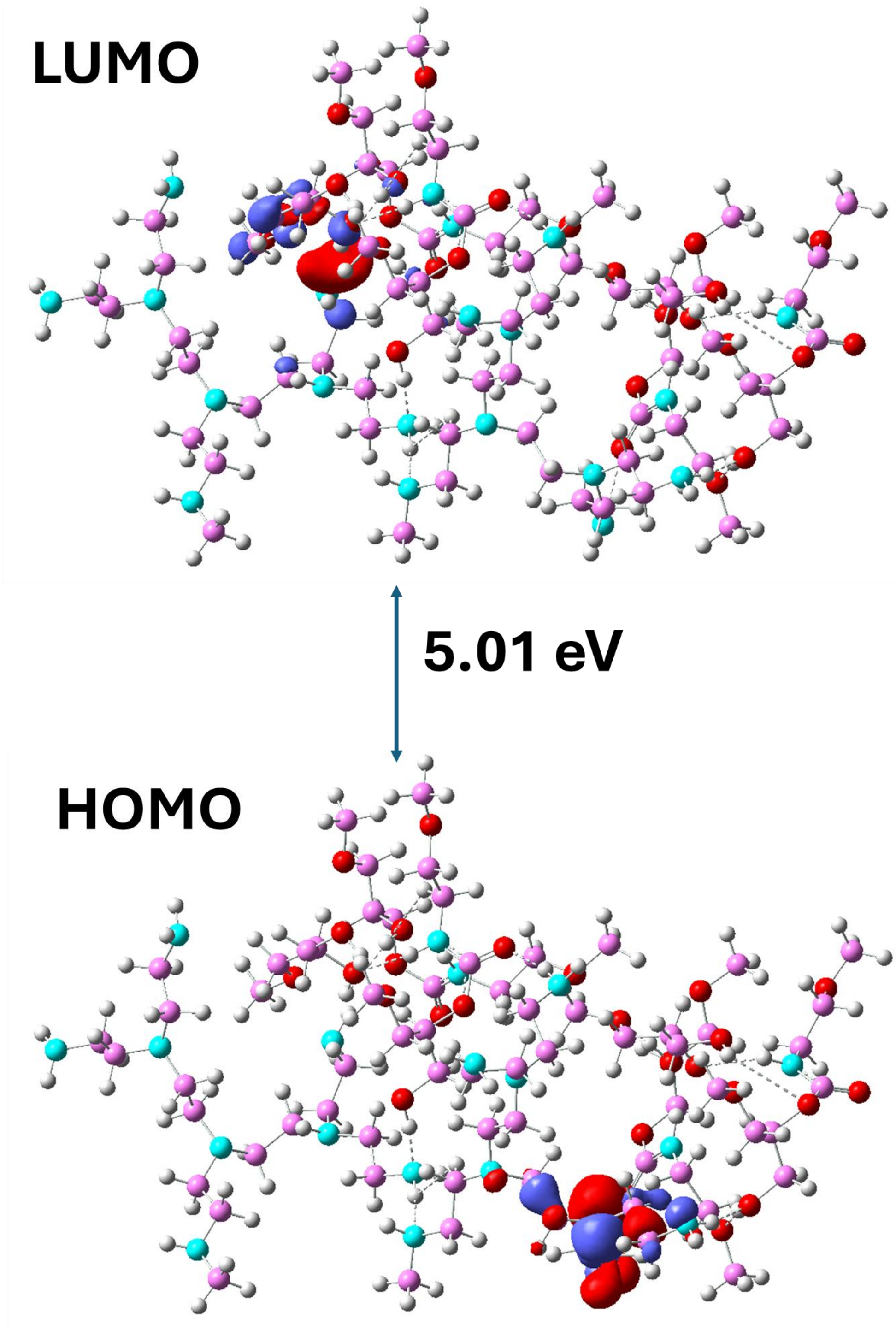


Figure S10. HOMO and LUMO of moderate aggregate (2 x (1+2+3+PEI))

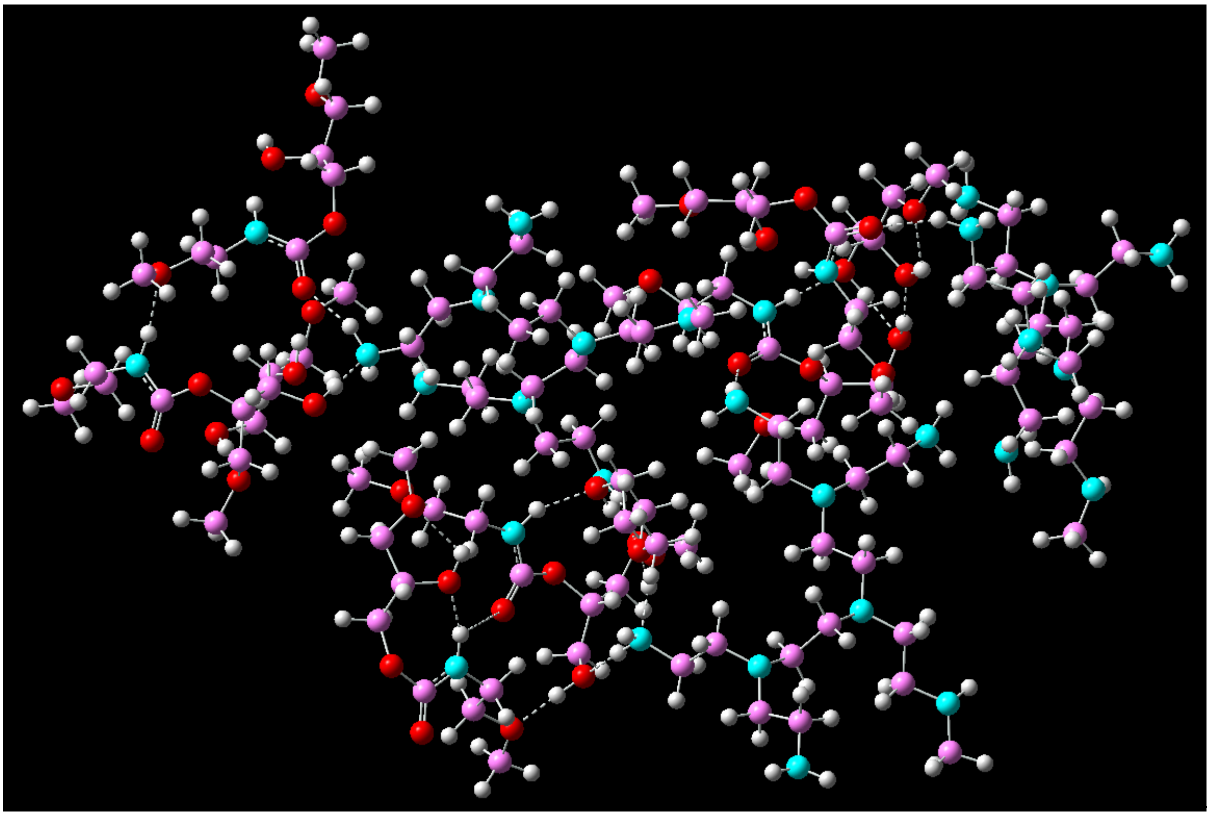


Figure S11. Optimized structure of large aggregate (3 x (1+2+3+PEI)) showing intra molecular hydrogen bonding interactions

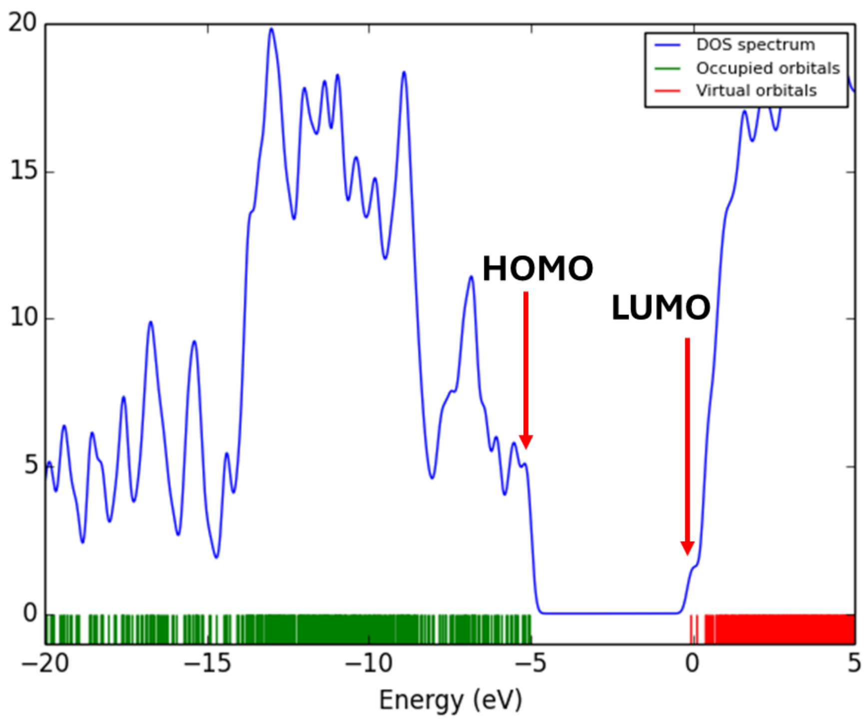


Figure S12. Density of state spectrum of large aggregate (3 x (1+2+3+PEI)) using B3LYP/6-311 level in the range of -20 to 5 eV

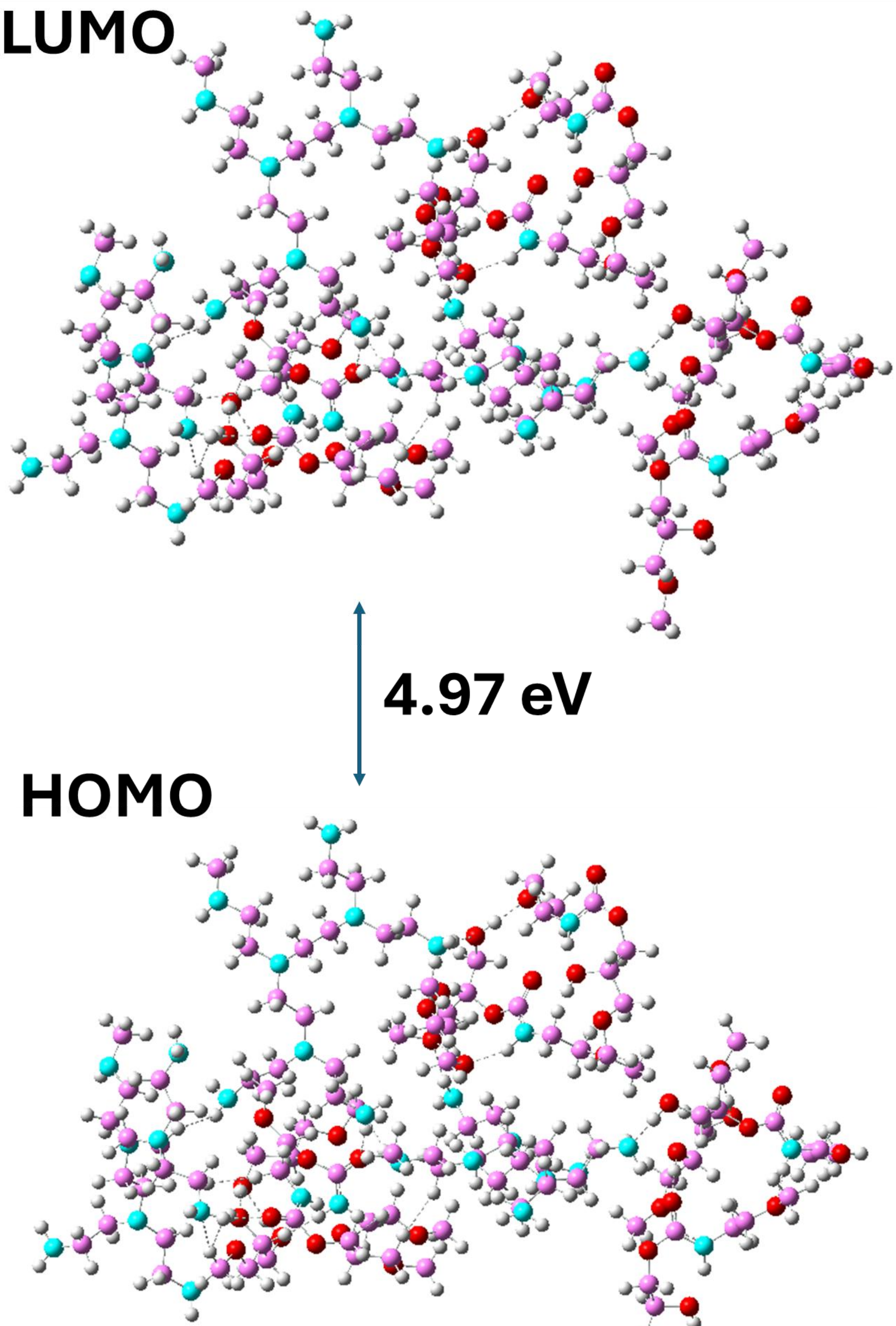


Figure S13. HOMO and LUMO energy difference of large aggregate (3 x (1+2+3+PEI))

FILM results of NIPU films

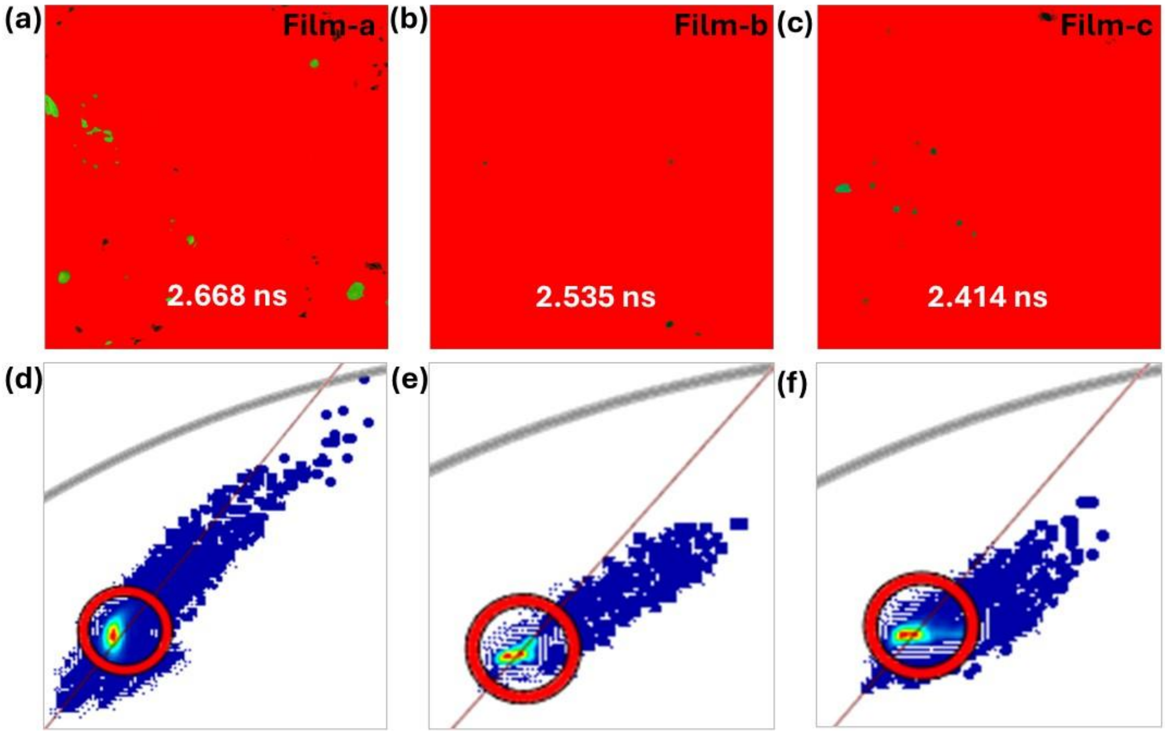
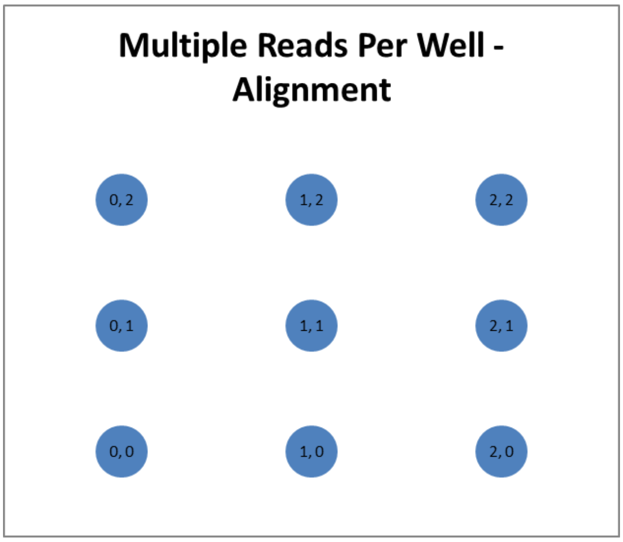


Figure S14. Fluorescence lifetime imaging microscopy (FLIM) images of (a) film-a, (b) film-b and (c) film-c using the laser source of 440 nm, height x width = 1024 x 2024; phasor histogram plots of NIPU (d) film-a, (e) film-b and (f) film-c showing lifetimes of 2.668, 2.535 and 2.414 ns, respectively; the curved grey line corresponds to the universal circle highlighting all possible phasors for monoexponential decays.

5. Humidity sensing by NIPU film-b

Fluorescence measurement for humidity sensing study by film-b

The fluorescence of water absorbed film-b (thickness = 0.44±0.005 mm) taking from different humidity chambers (10-85%) were recorded at 520 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 450 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, μclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 μs, 0 μs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced film-b. All the results were done twice with three replicates.



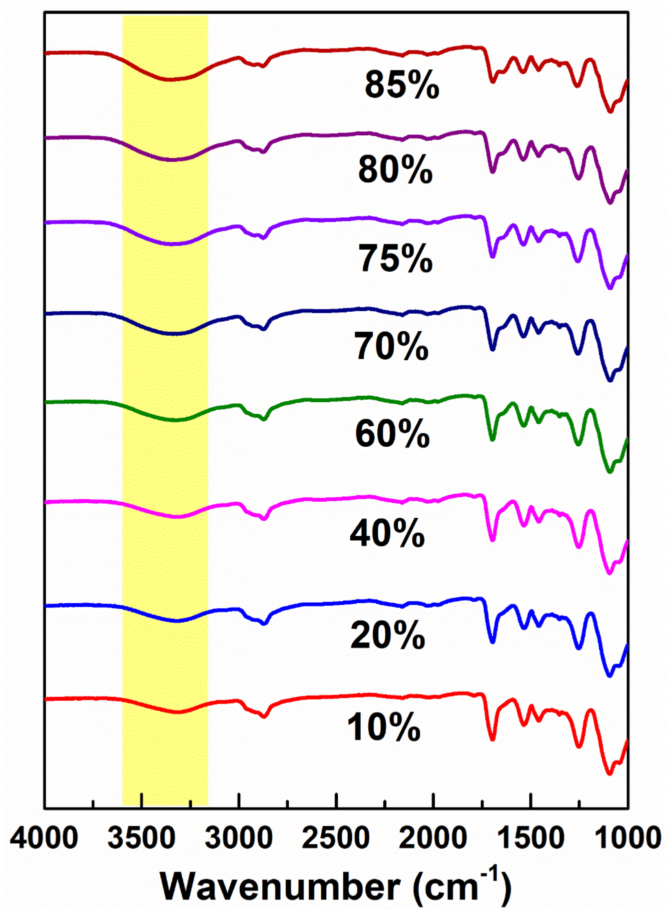


Figure S15. ATR-infrared spectra of NIPU film-b at 10%, 20%, 40% and 60% RH 70%, 75%, 80% and 85% RH

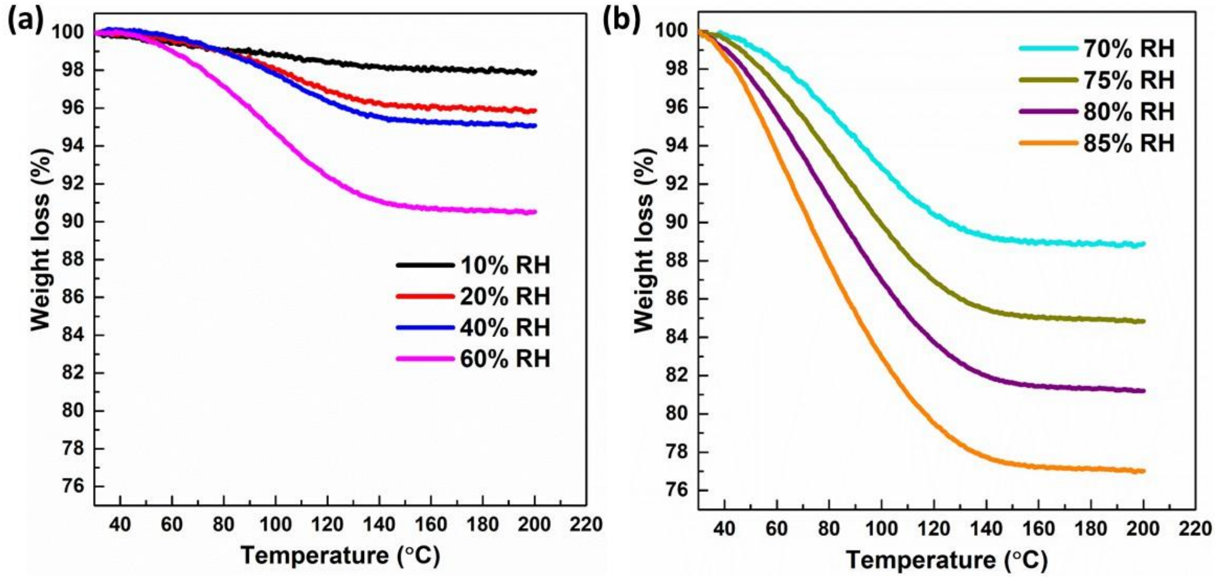


Figure S16. TGA thermograms of NIPU film-b at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

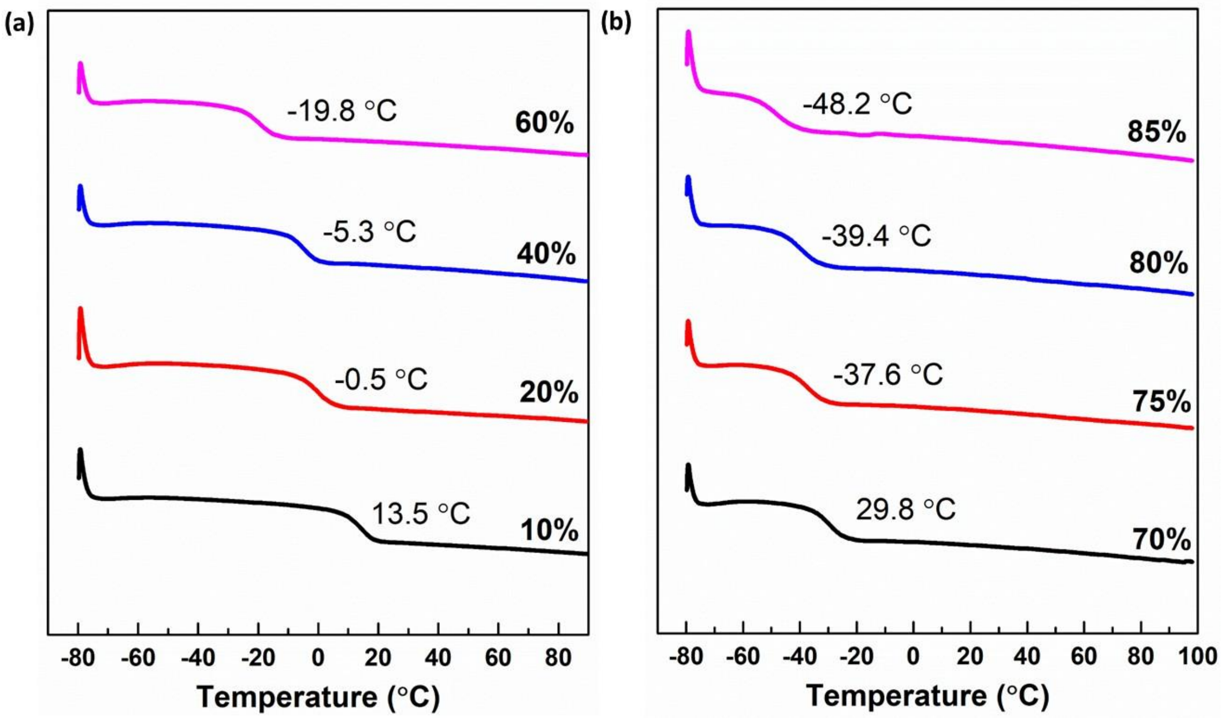


Figure S17. DSC thermograms of NIPU film-b at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

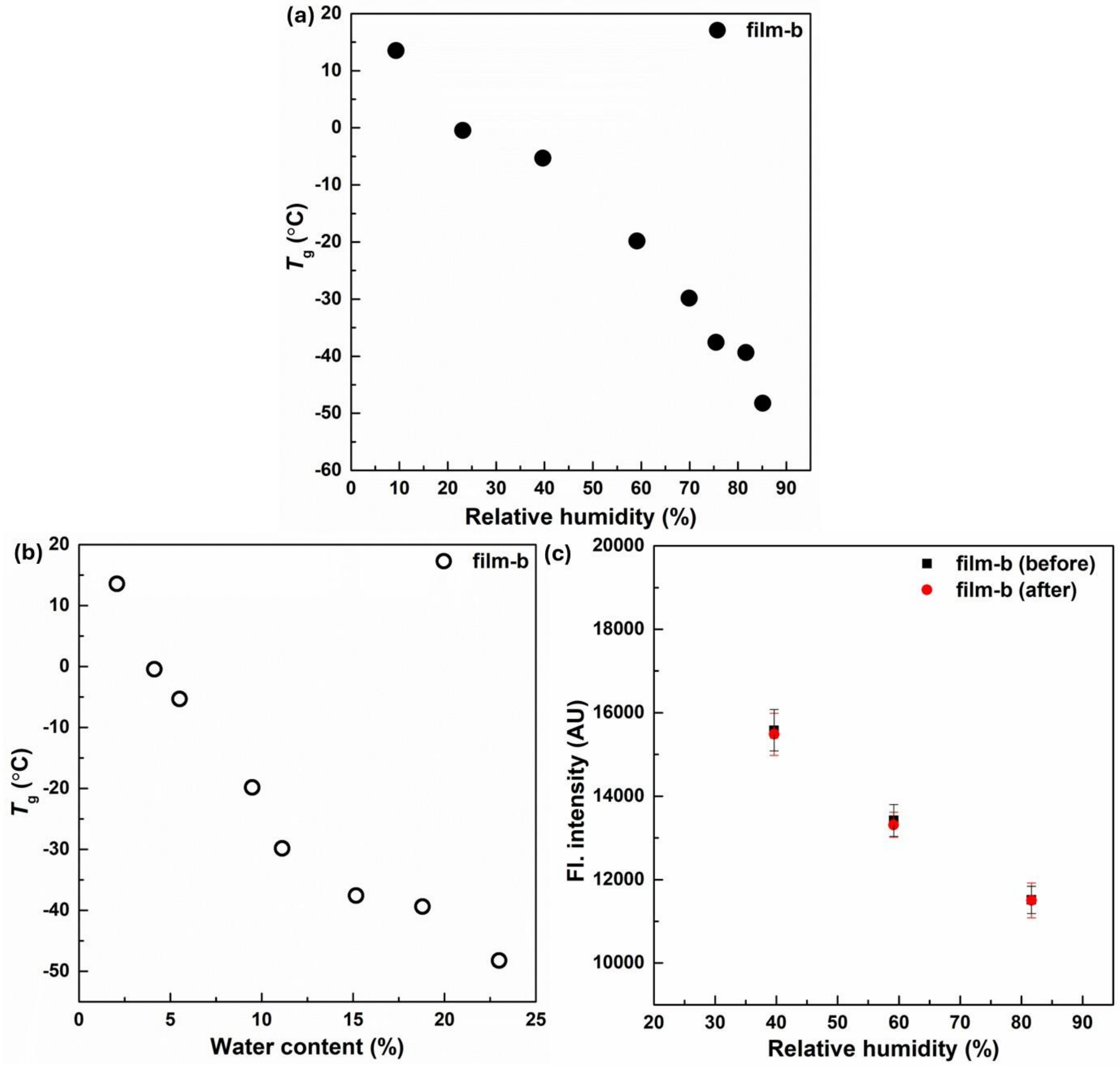


Figure S18. The plots T_g versus (a) % relative humidity and (b) water content of NIPU film-b; (c) fluorescence reversibility test of NIPU film-b at 40%, 60%, and 80% RHs (see section 1.5.5. for experimental details)

6. pH sensitivity and stability of the NIPU film

The pH sensitivity and stability of the NIPU films were evaluated under various acidic conditions (pH = 6.8, 4.8, 4.1, and 2.6), prepared by adjusting CH_3COOH and NaOH concentrations. The films were immersed in these solutions for 24 h, subsequently removed, air-dried for 4 h, and then vacuum-dried at 80 °C for 24 h. The treated samples were characterized by ATR-Infrared, differential scanning calorimetry (DSC), fluorescence spectroscopy, and scanning electron microscope (SEM), and their properties/ morphologies were compared with those of the pristine NIPU film. However, no noticeable properties or morphological changes were observed, as shown in Figure S19-S20.

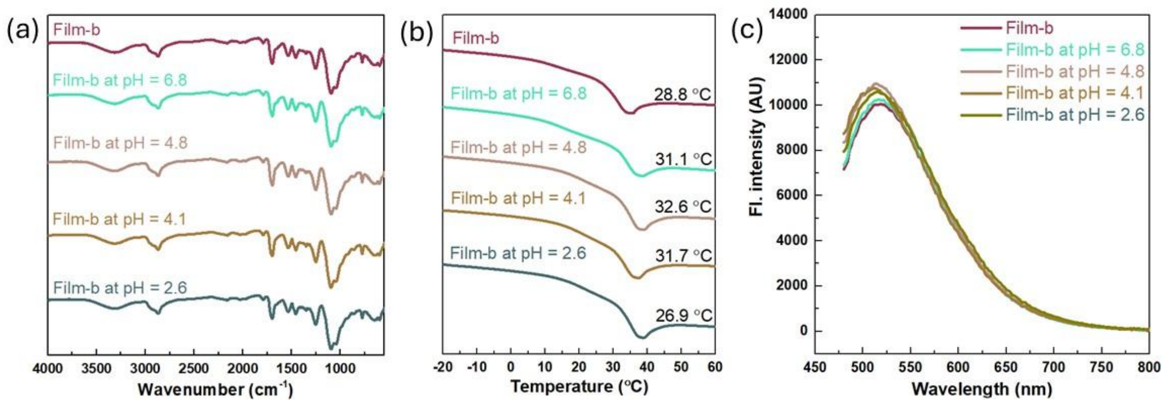


Figure S19. (a) ATR-Infrared spectra of film-b, (b) DSC plots of film-b, and (c) fluorescence spectra of film-b using excitation wavelength of 450 nm after immersion at different pH (6.8, 4.8, 4.1, and 2.6) for 24 h and subsequent drying

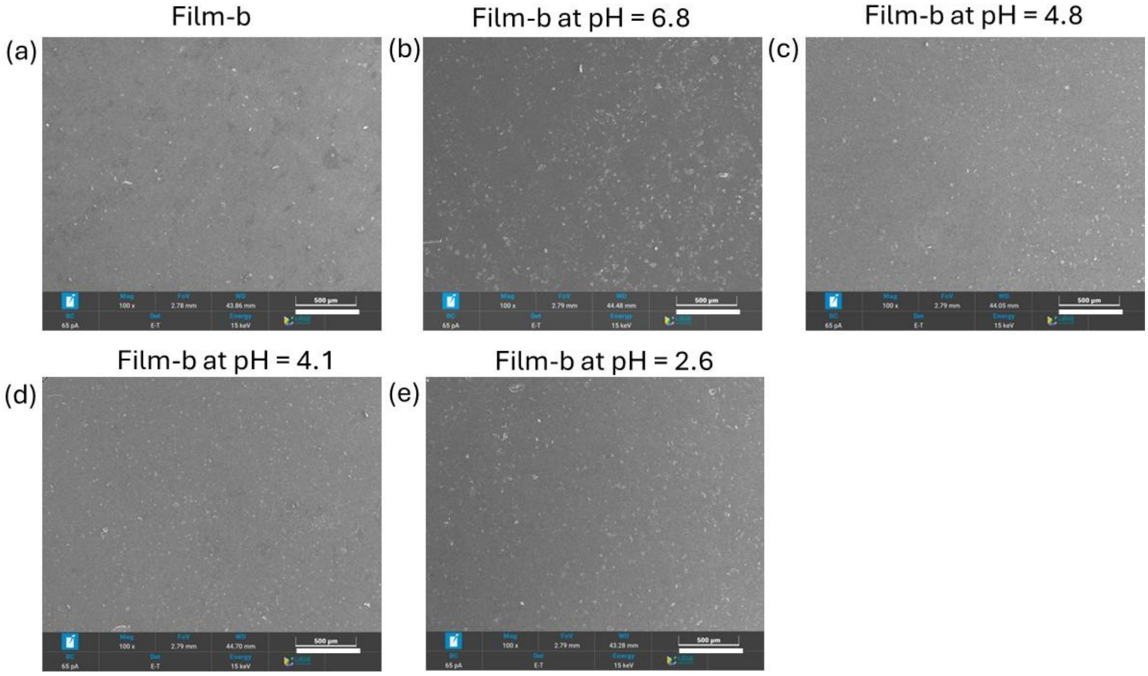


Figure S20. SEM images of (a) film-b and SEM images of film-b after immersion at different pH (b) 6.8, (c) 4.8, (d) 4.1, and (e) 2.6 for 24 h and subsequent drying

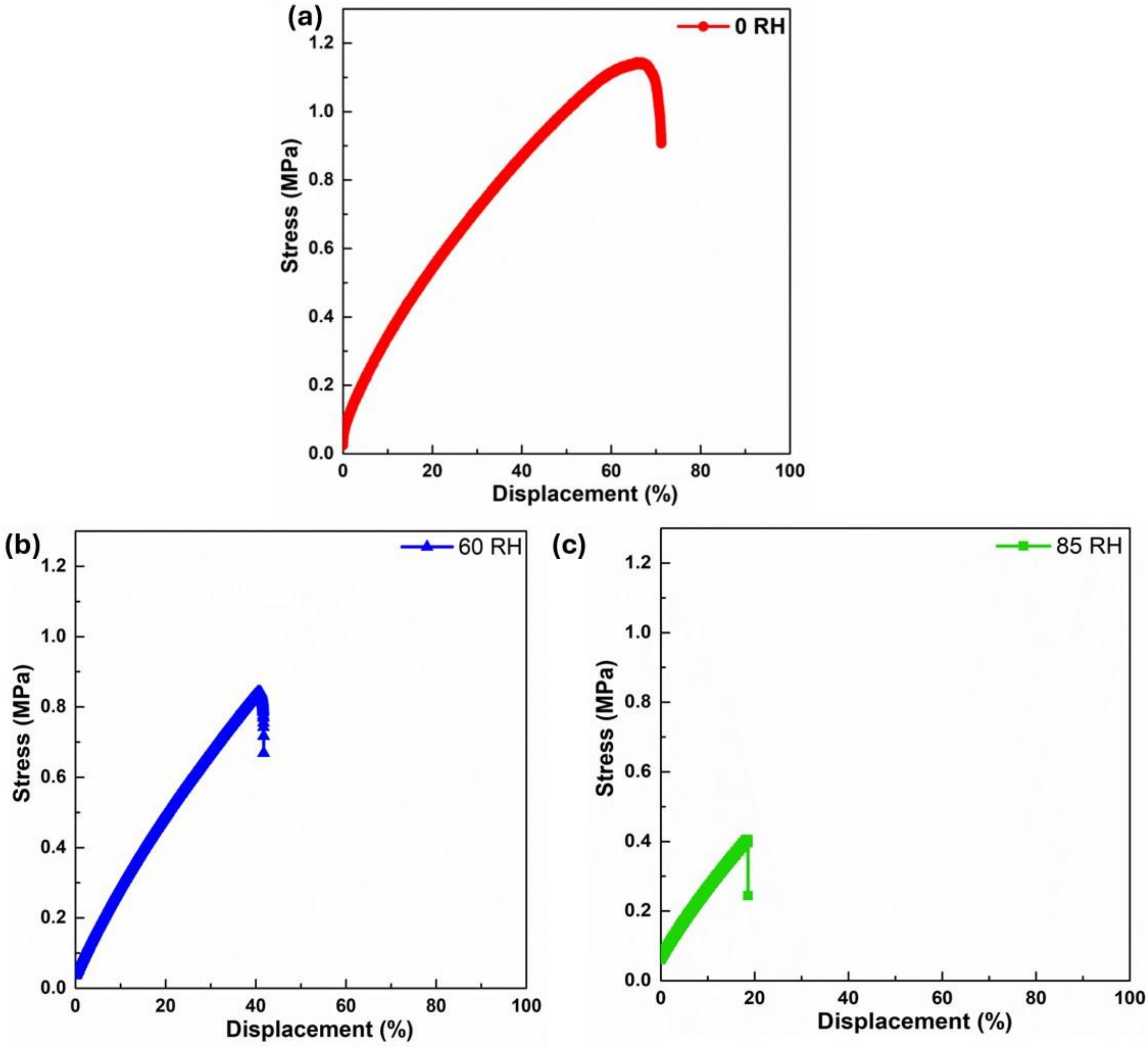


Figure S21. The stress versus %displacement plots of NIPU film-b at (a) 0%, (b) 60% and (c) 85% of relative humidity

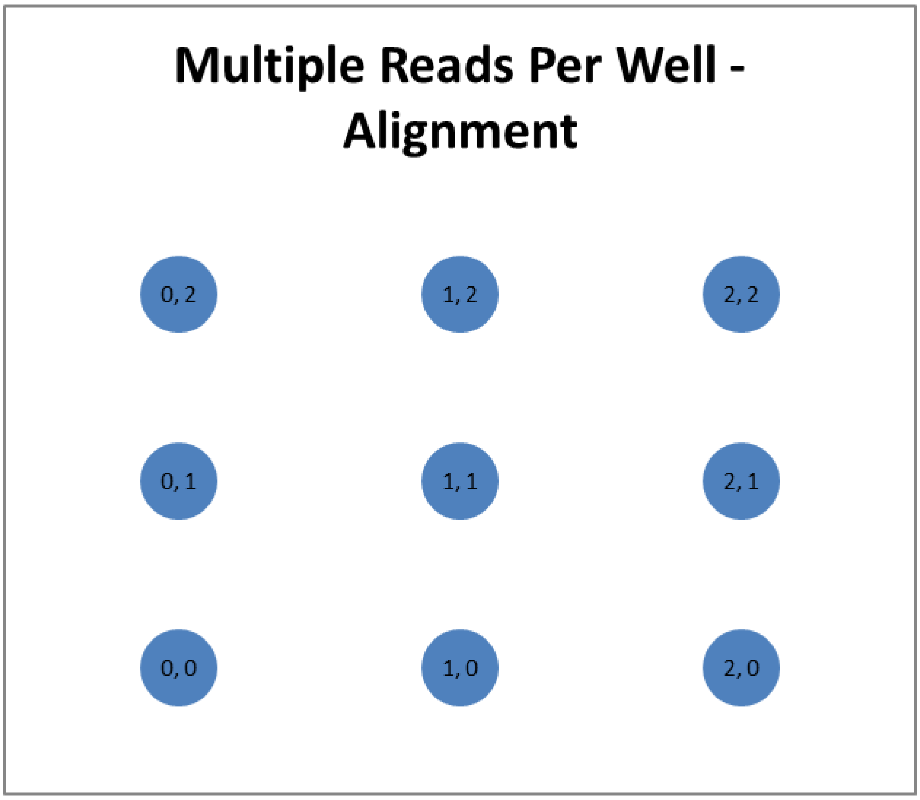
Table S5: Mechanical properties of NIPU film-b

Relative humidity (%)	Young modulus (MPa)	Elongation at break (%)	Stress at break (MPa)
0	2.83±0.12	67.2	1.14
60	2.64±0.11	40.7	0.84
85	1.60±0.46	18.5	0.41

7. Humidity sensing by NIPU film-a

Fluorescence measurement for humidity sensing study by film-a

The fluorescence of water absorbed film-a (thickness = 0.43±0.01 mm) taking from different humidity chambers (10-85%) were recorded at 490 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 430 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, µclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 µs, 0 µs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced film-a. All the results were done twice with three replicates.



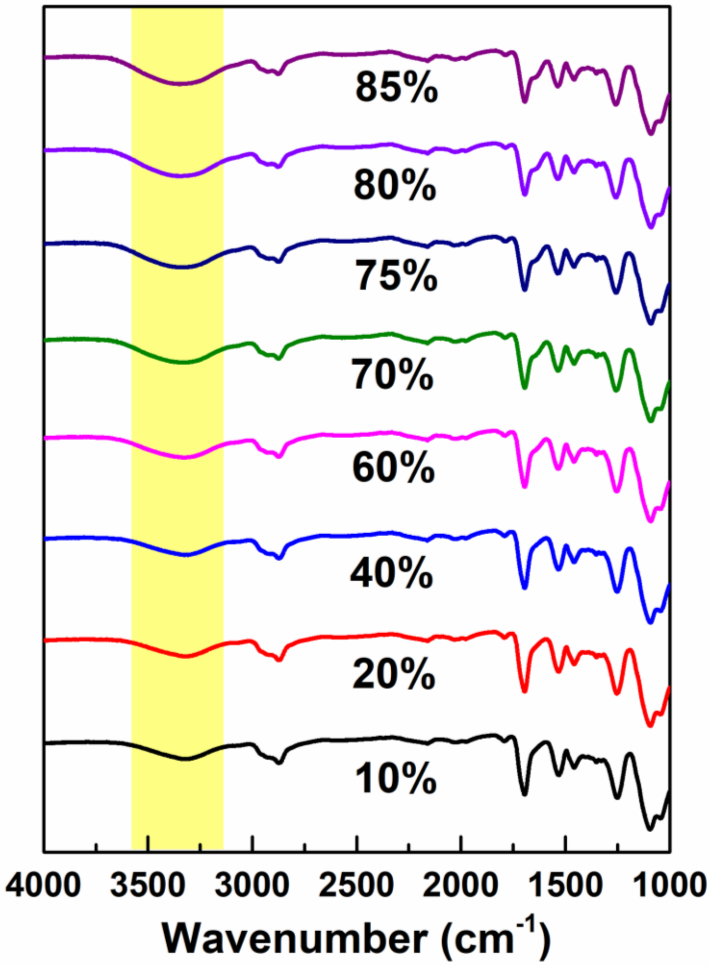


Figure S22. ATR-infrared spectra of NIPU film-a at 10%, 20%, 40%, 60%, 70%, 75%, 80% and 85% relative humidity

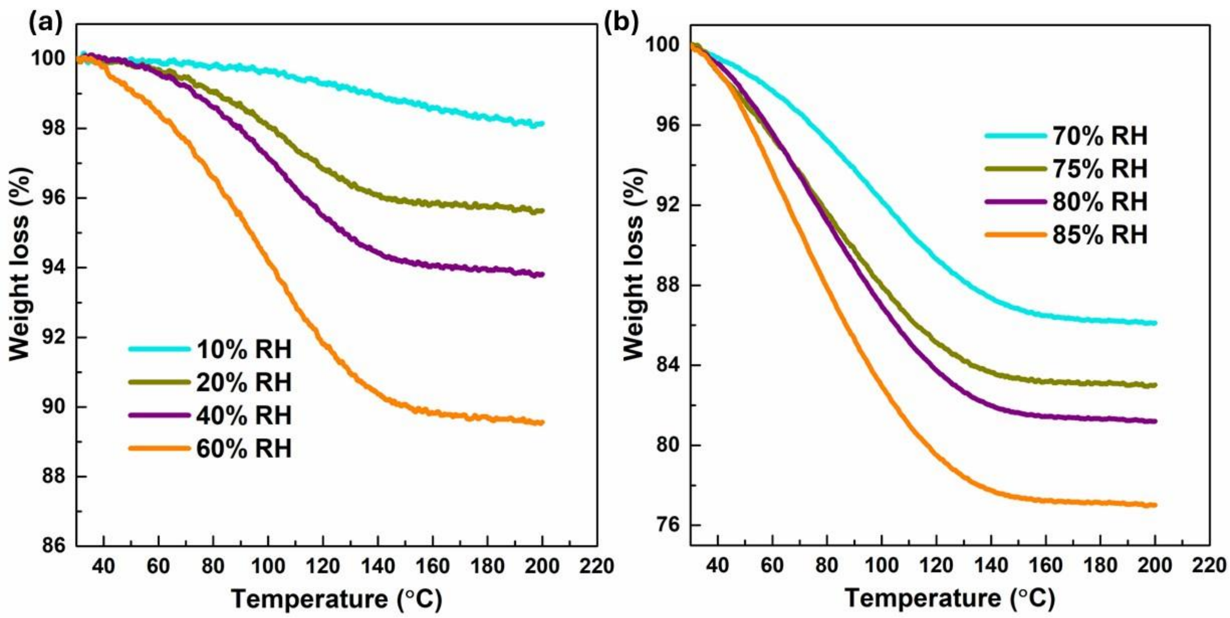


Figure S23. TGA thermograms of NIPU film-a at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

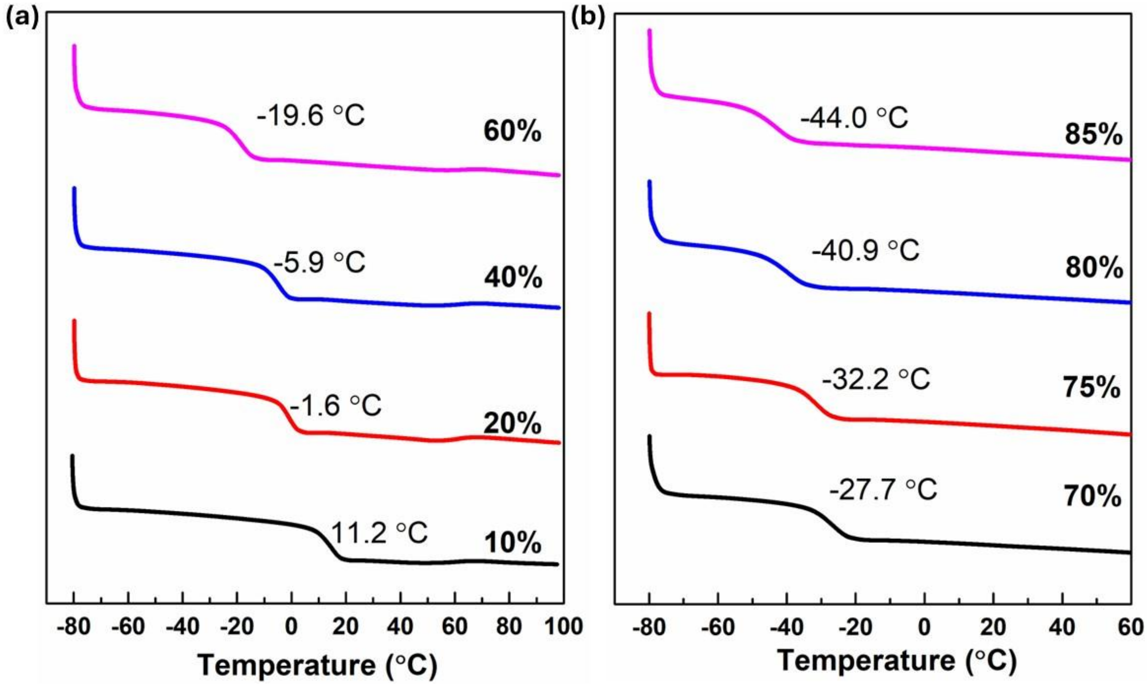


Figure S24. DSC thermograms of NIPU film-a at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

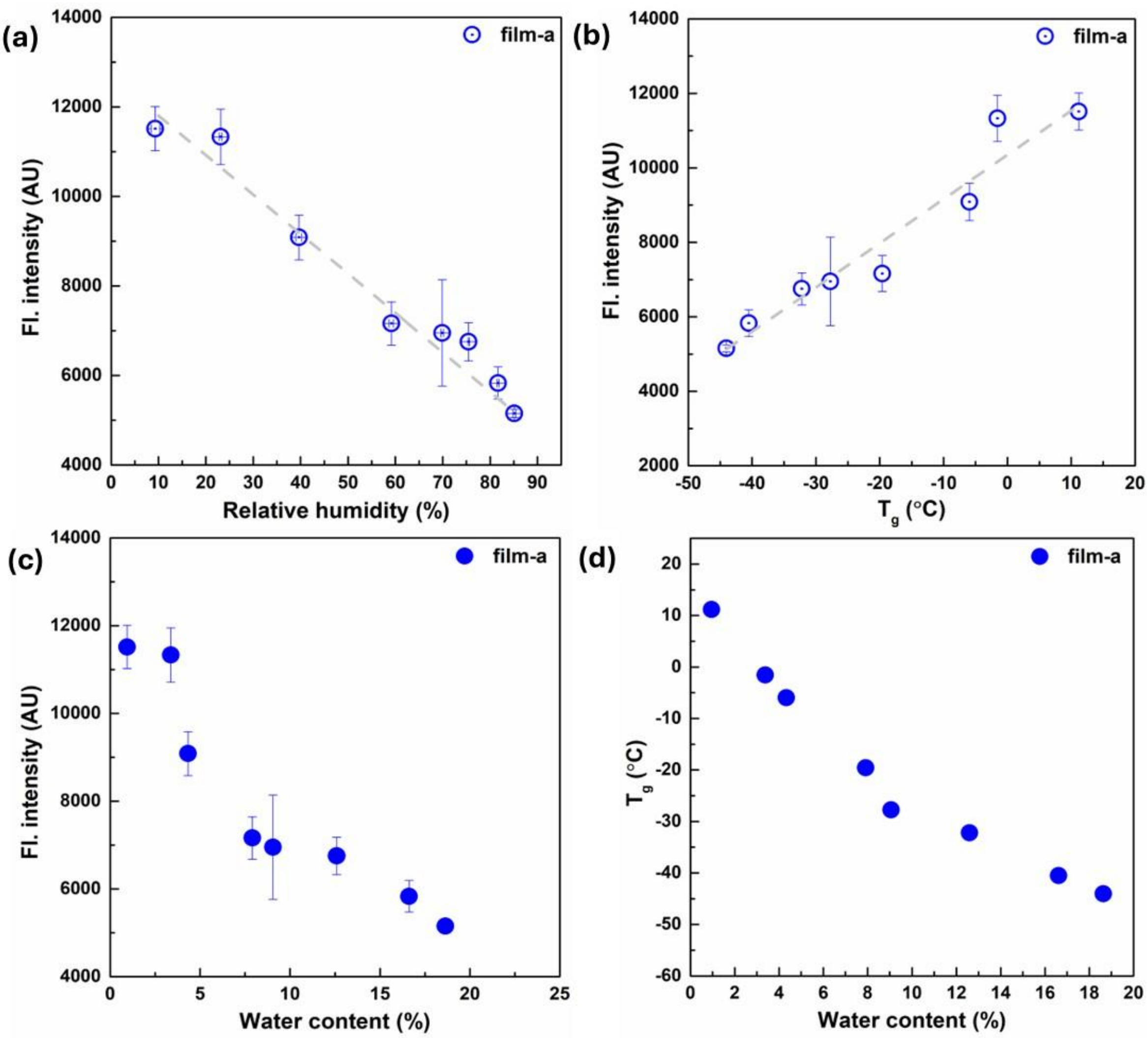
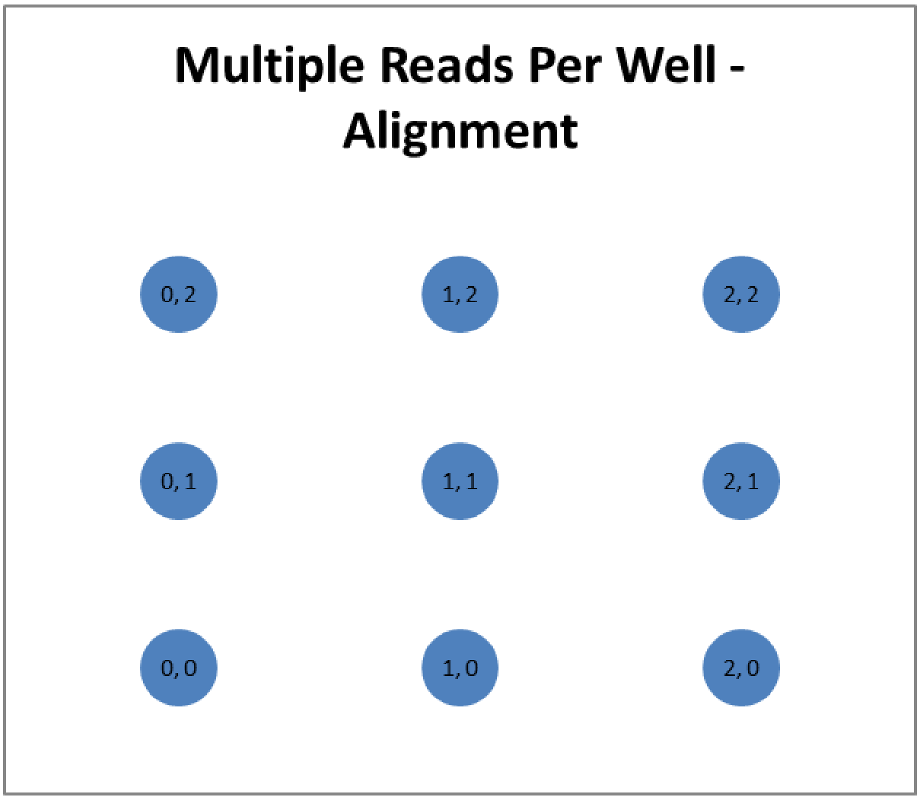


Figure S25. (a) The linear changes in fluorescence intensity of NIPU film-a with relative humidity and (b) the change in fluorescence intensity of NIPU film-a with T_g; (c) the plot of fluorescence intensity of NIPU film-a with water contents; (d) the plot of T_g of NIPU film-a with water contents

8. Humidity sensing by NIPU film-c

Fluorescence measurement for humidity sensing study by film-c

The fluorescence of water absorbed film-c (thickness = 0.40±0.005 mm) taking from different humidity chambers (10-85%) were recorded at 552 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 490 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, µclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 µs, 0 µs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced film-c. All the results were done twice with three replicates.



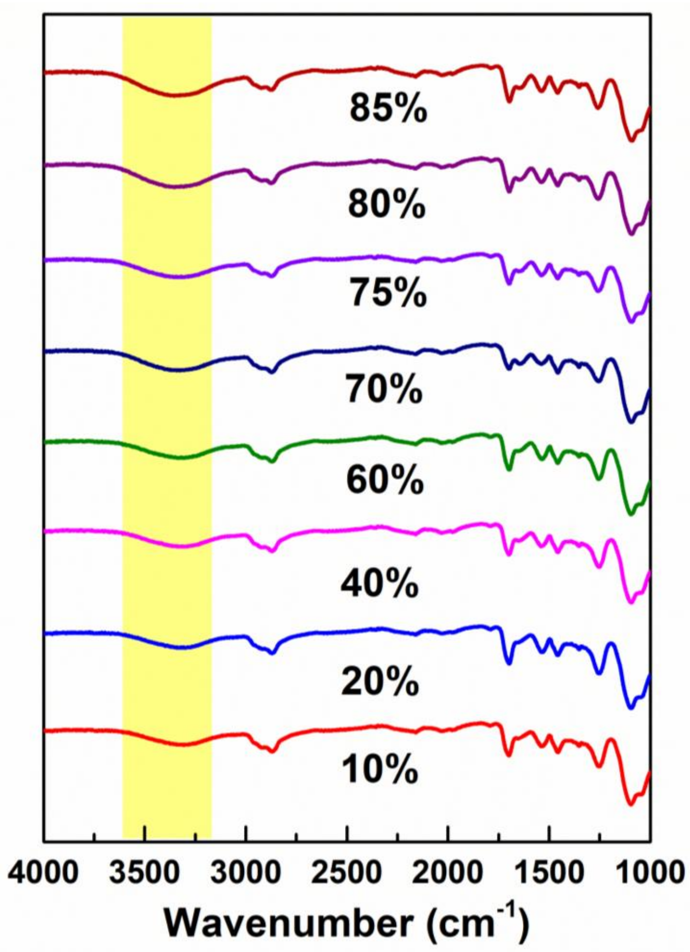


Figure S26. ATR-infrared spectra of NIPU film-c at 10%, 20%, 40% and 60% RH 70%, 75%, 80% and 85% RH

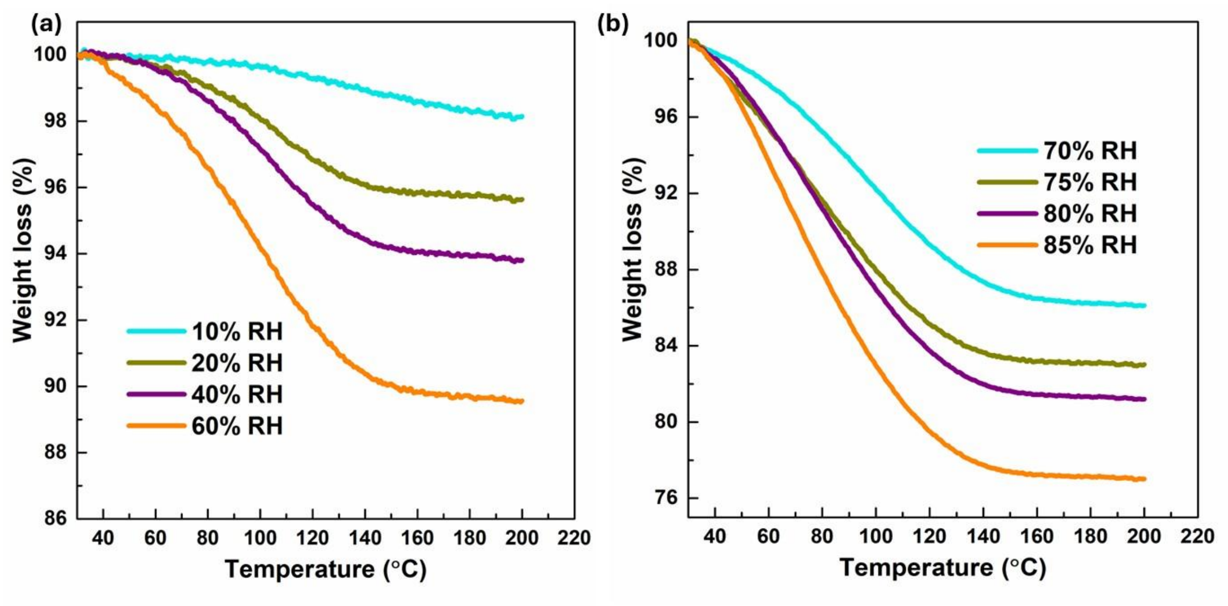


Figure S27. TGA thermograms of NIPU film-c at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

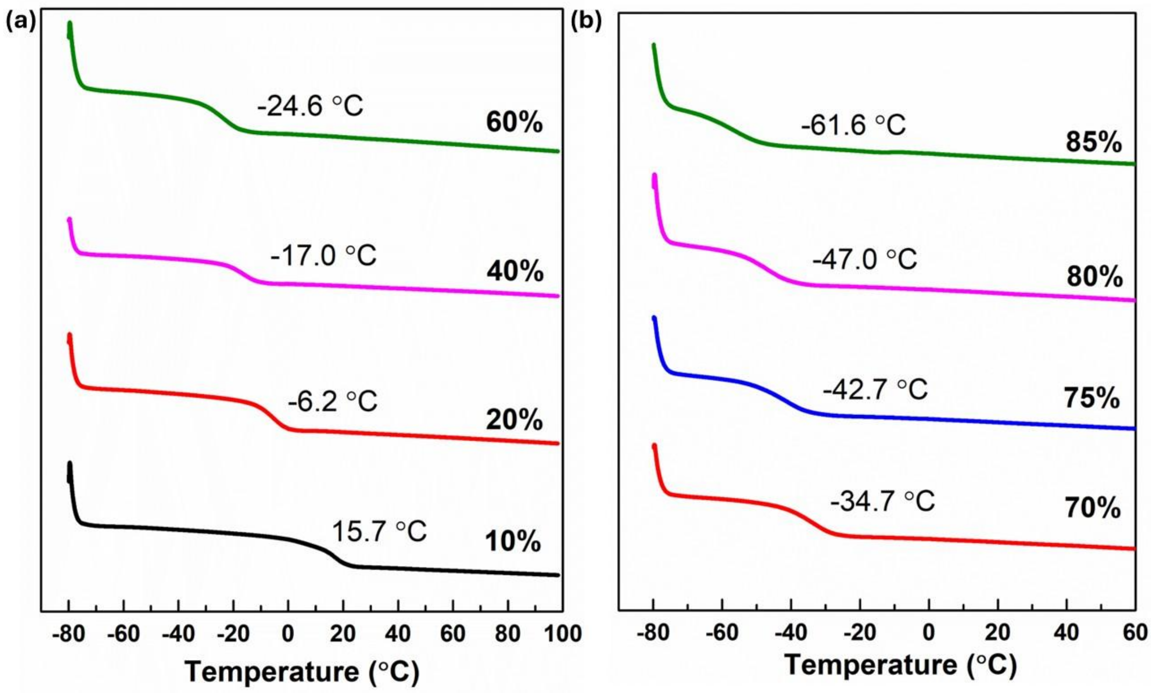


Figure S28. DSC thermograms of NIPU film-c at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

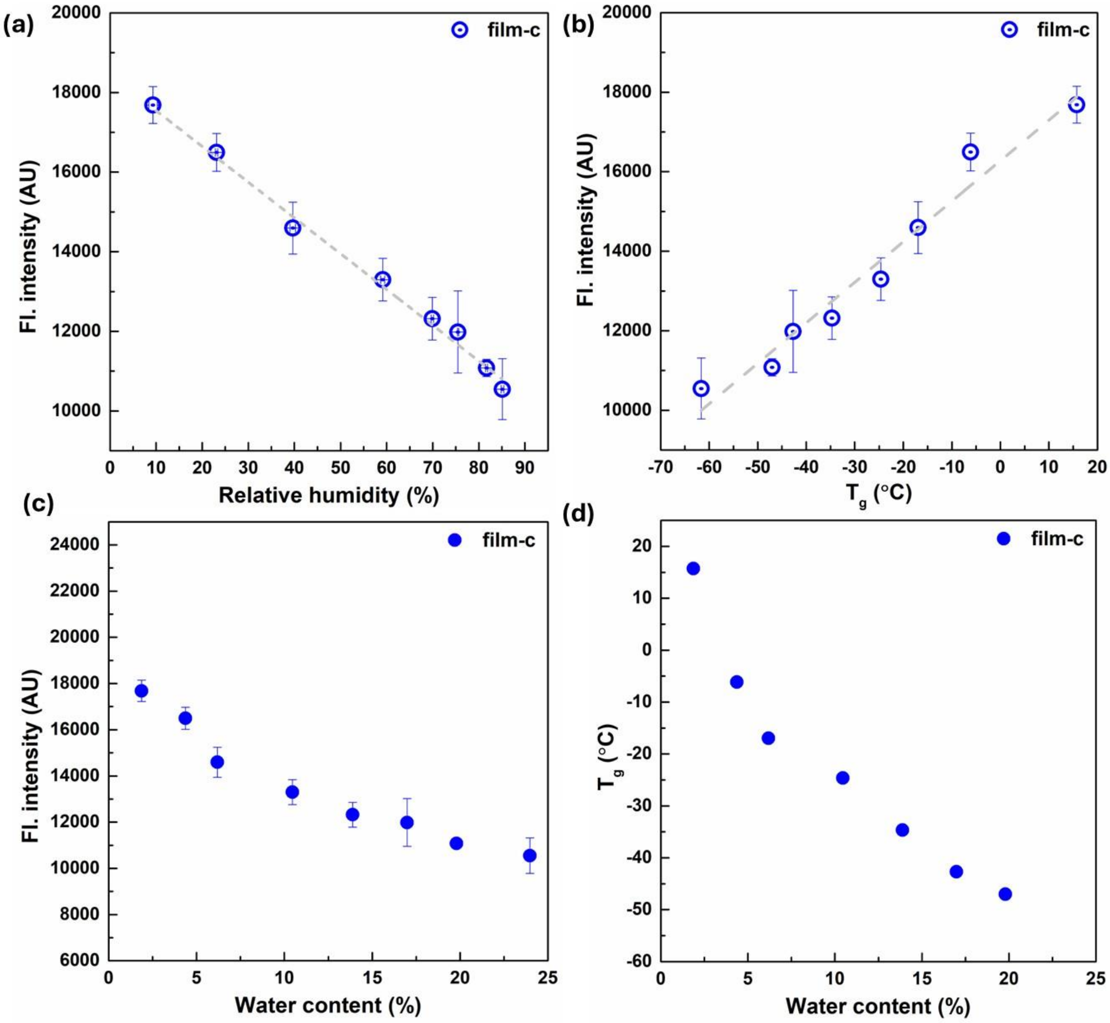
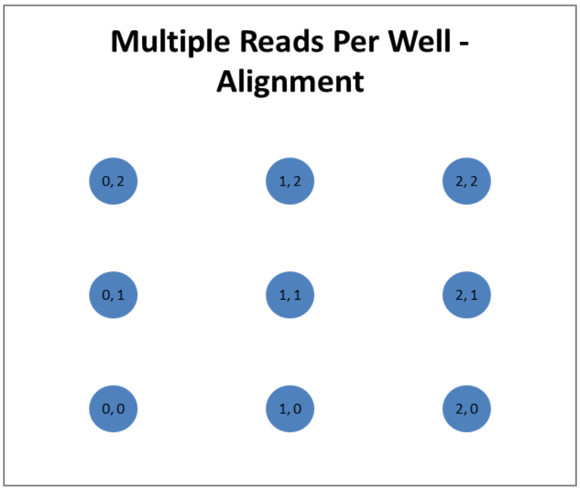


Figure S29. (a) The linear changes in fluorescence intensity of NIPU film-c with relative humidity and (b) the change in fluorescence intensity of NIPU film-c with T_g; (c) the plot of fluorescence intensity of NIPU film-c with water contents; (d) the plot of T_g of NIPU film-c with water content (%)

9. Humidity sensing by non-foamed NIPU

Fluorescence measurement for humidity sensing study by non-foamed NIPU

The fluorescence of water absorbed non-foamed NIPUs (thickness = 1.50±0.02 mm) taking from different humidity chambers (10-85%) were recorded at 486 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 430 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, μclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 μs, 0 μs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured from different portions (as shown below) of introduced non-foamed NIPU. All the results were done twice with three replicates.



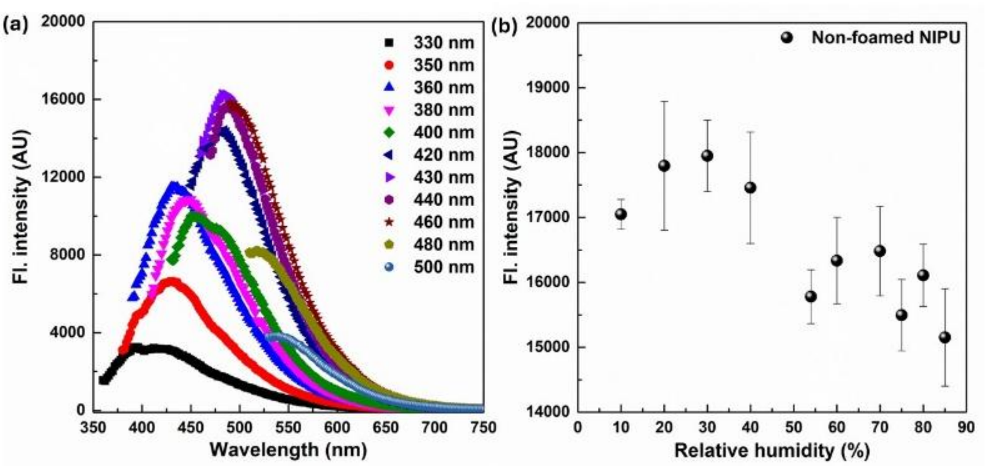
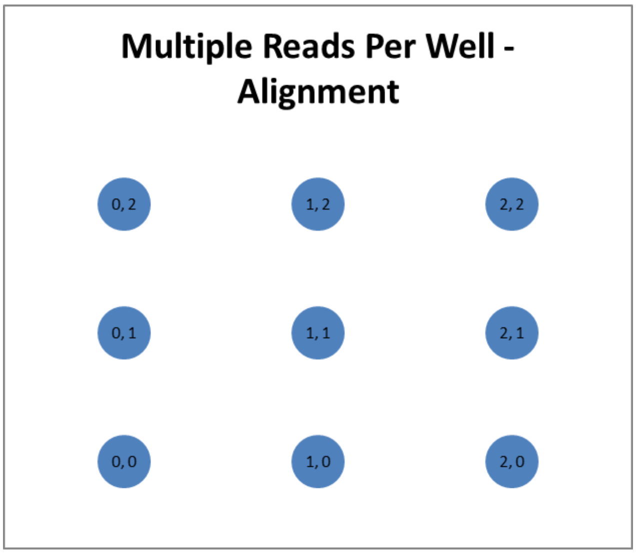


Figure S30. (a) Excitation-dependent emission of non-foamed NIPU within 330-500 nm and (b) change of fluorescence intensity of non-foamed NIPU with different RH (10-85%)

10. Humidity sensing by NIPU film containing 1,3-bis(aminomethyl)cyclohexane (BAC)

Fluorescence measurement for humidity sensing study by film containing BAC

The fluorescence of water absorbed films containing BAC (thickness = 0.44±0.005 mm) taking from different humidity chambers (10-85%) were recorded at 505 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 460 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, µclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 µs, 0 µs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced film containing BAC. All the results were done twice with three replicates.



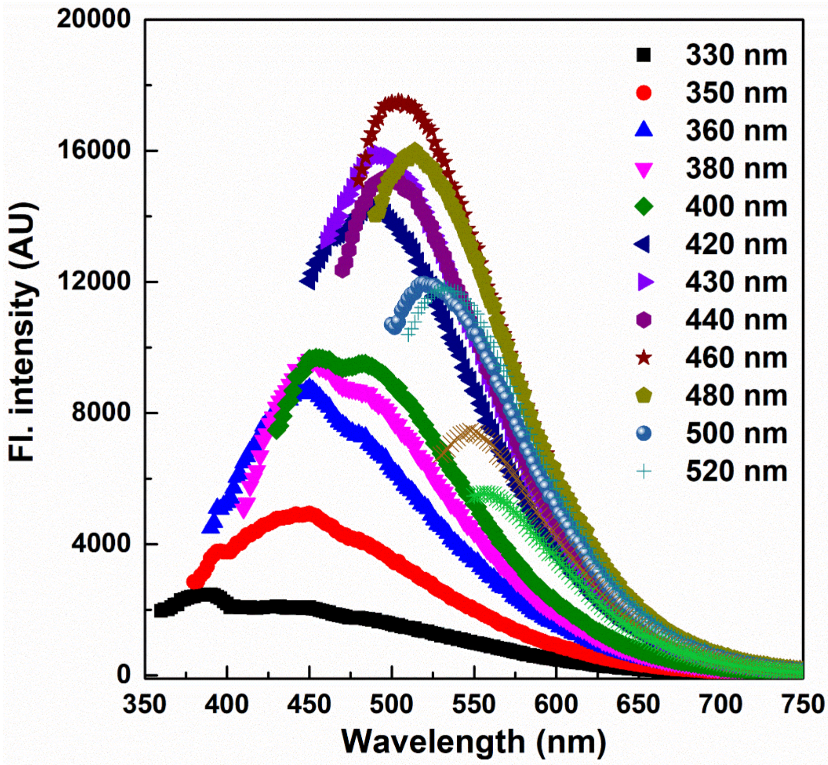


Figure S31. Excitation-dependent emission of NIPU film comprising 1,3-bis(aminomethyl)cyclohexane

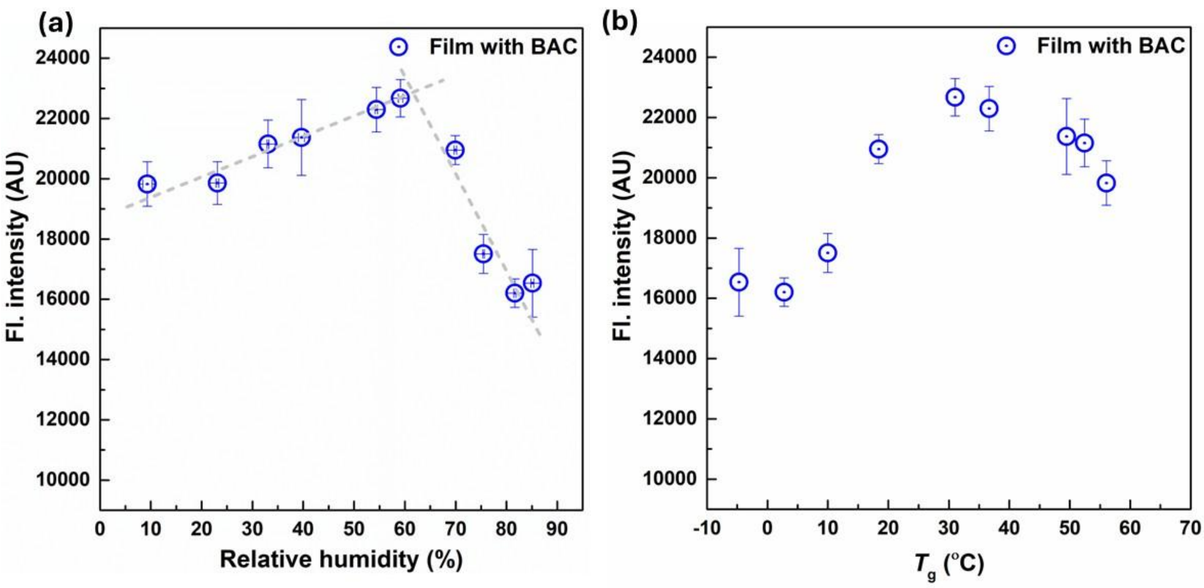


Figure S32. Change of fluorescence intensity of NIPU film containing 1,3-bis(aminomethyl)cyclohexane with (a) different RH (10-85%) and (b) T_g

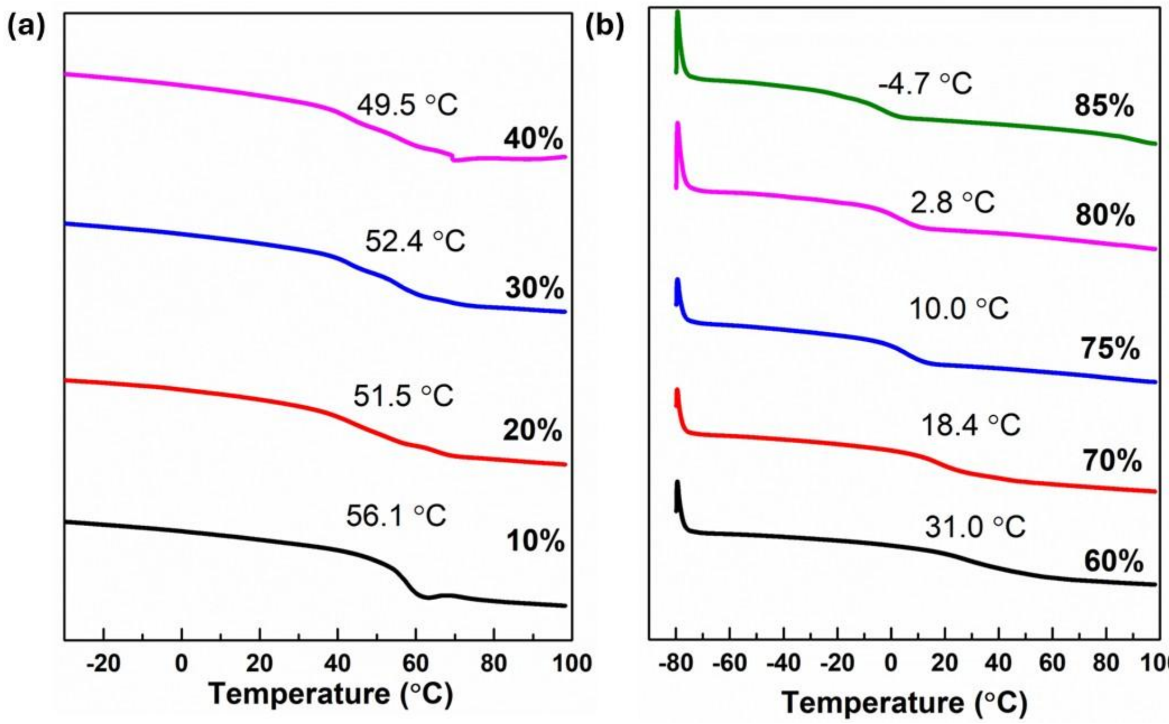


Figure S33. DSC thermograms of NIPU films containing 1,3-bis(aminomethyl)cyclohexane at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

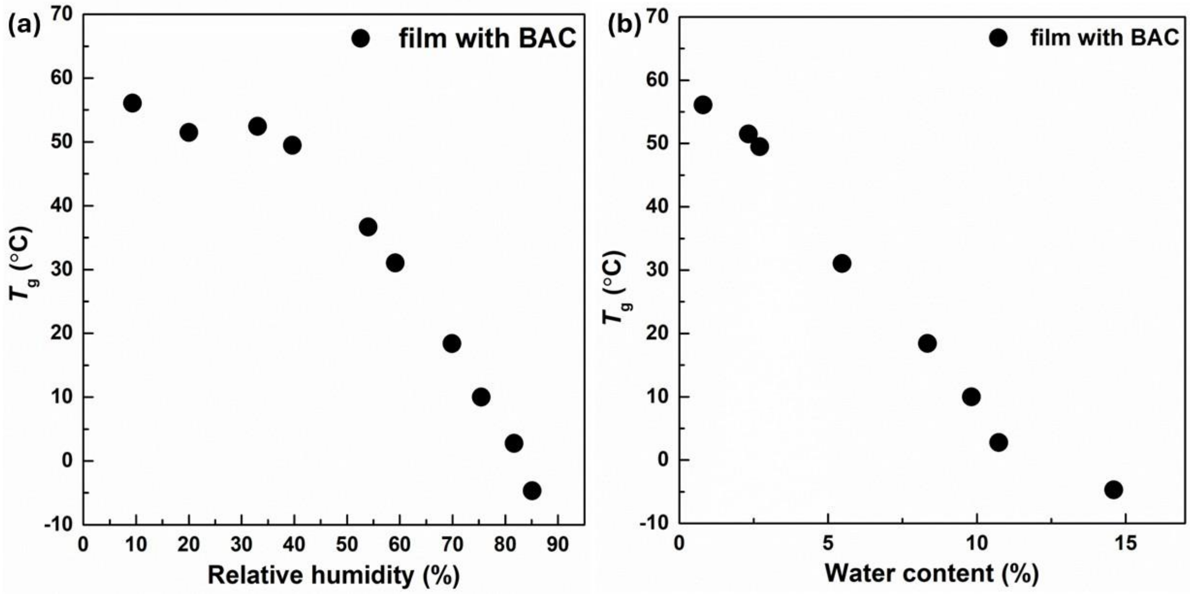


Figure S34. DSC thermograms of NIPU films containing 1,3-bis(aminomethyl)cyclohexane at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

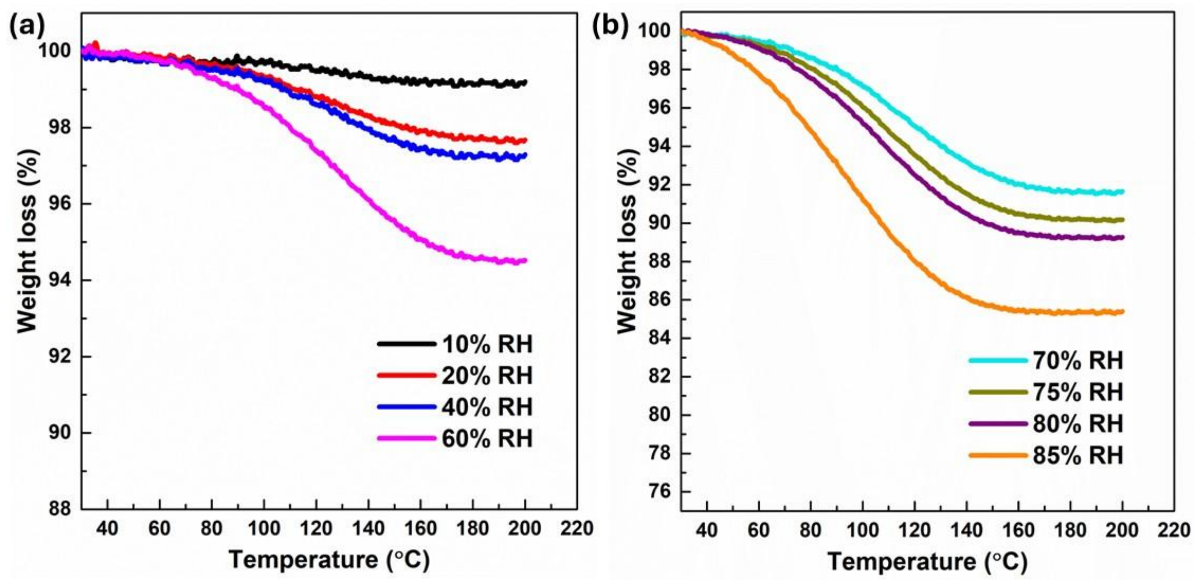


Figure S35. TGA thermograms of NIPU films containing 1,3-bis(aminomethyl)cyclohexane at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

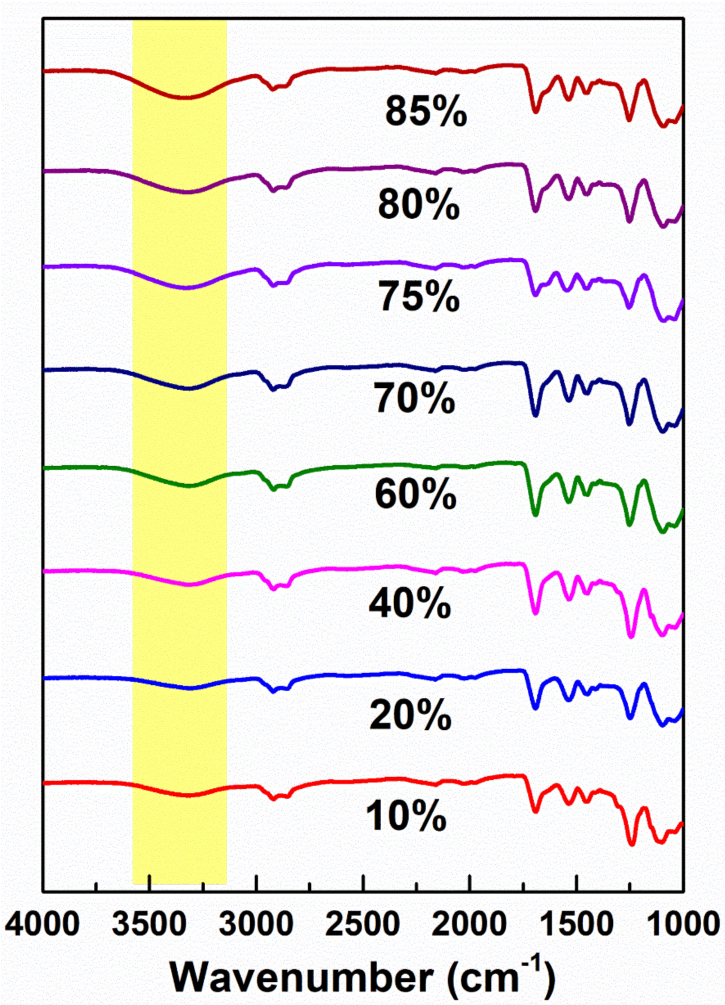
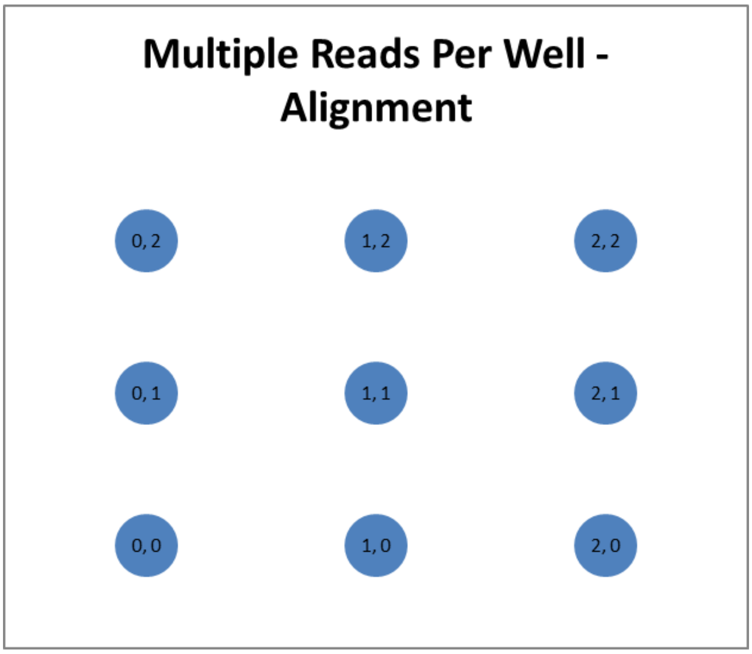


Figure S36. ATR-infrared spectra of NIPU film containing 1,3-bis(aminomethyl)cyclohexane at 10%, 20%, 40%, 60%, 70%, 75%, 80% and 85% RH

11. Humidity sensing by hybrid petro-based NIPU film

Fluorescence measurement for humidity sensing study by hybrid petro-based NIPU film

The fluorescence of water absorbed hybrid petro-based NIPU films (thickness = 0.46±0.008 mm) taking from different humidity chambers (10-85%) were recorded at 484 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 420 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, μclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 μs, 0 μs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced hybrid petro-based NIPU film. All the results were done twice with three replicates.



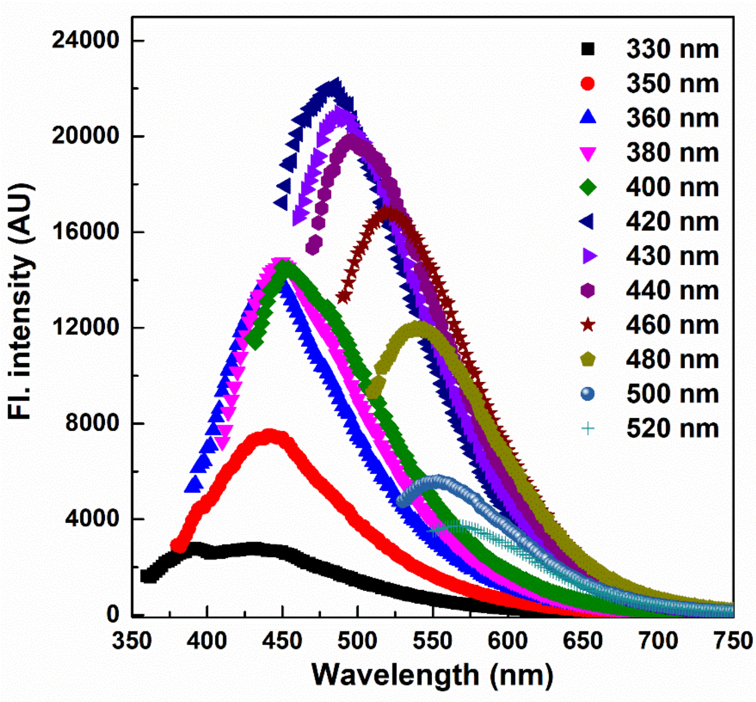


Figure S37. Excitation-dependent emission of hybrid petro-based NIPU film

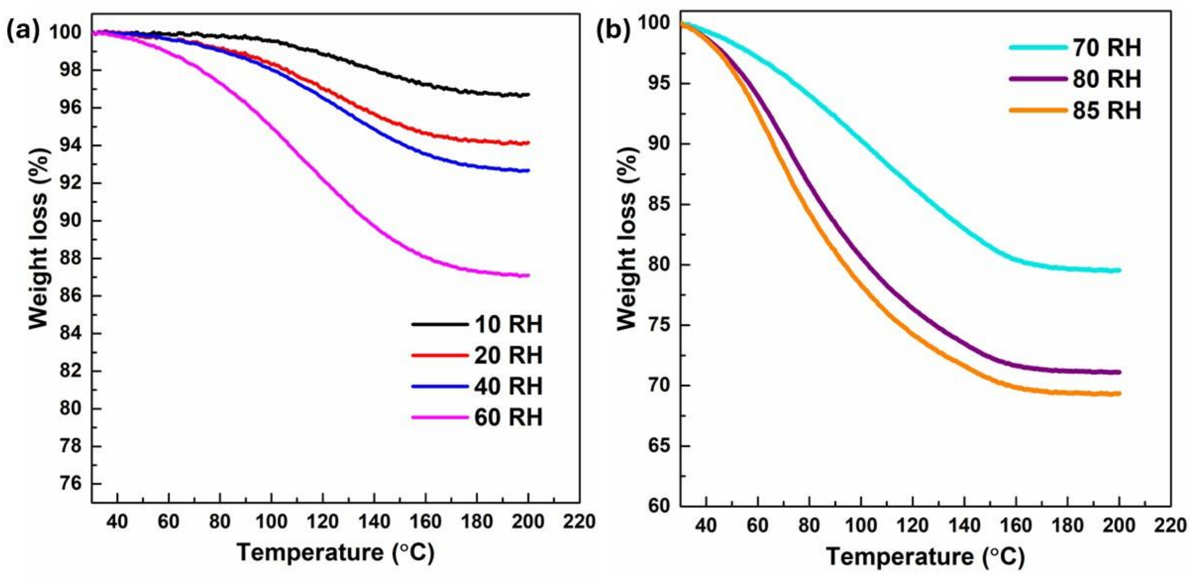


Figure S38. TGA thermograms of hybrid petro-based NIPU films at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 80% and 85% RH

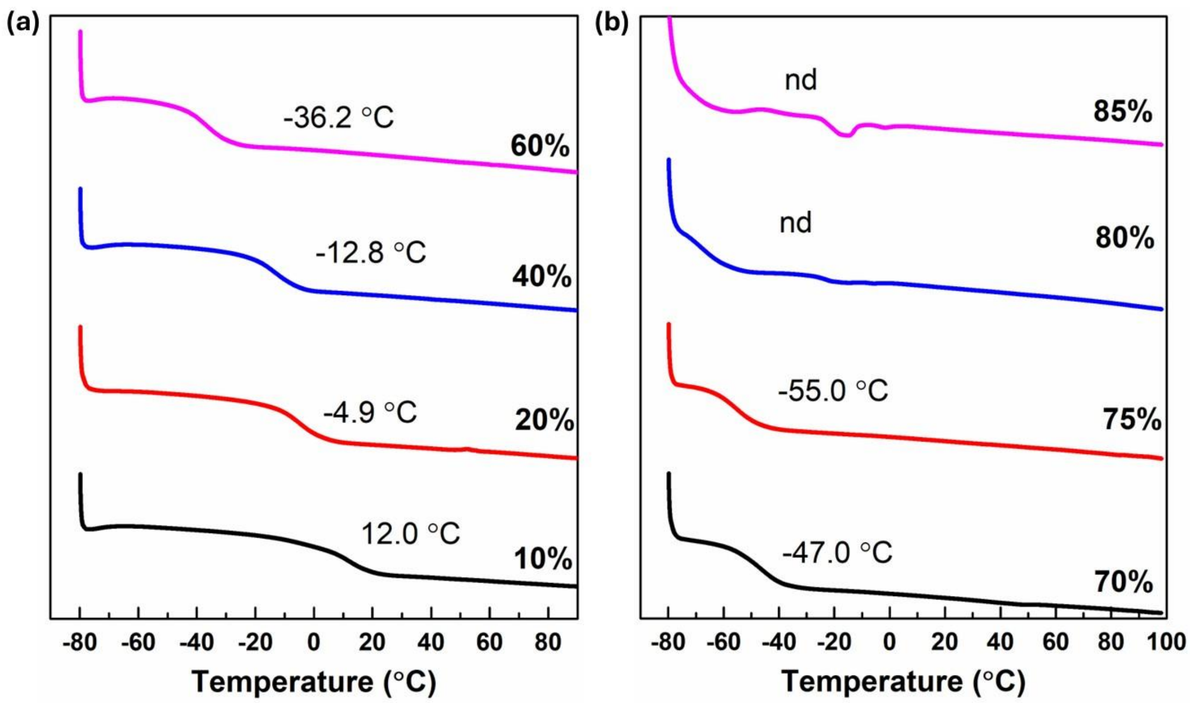


Figure S39. DSC thermograms of hybrid petro-based NIPU film at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

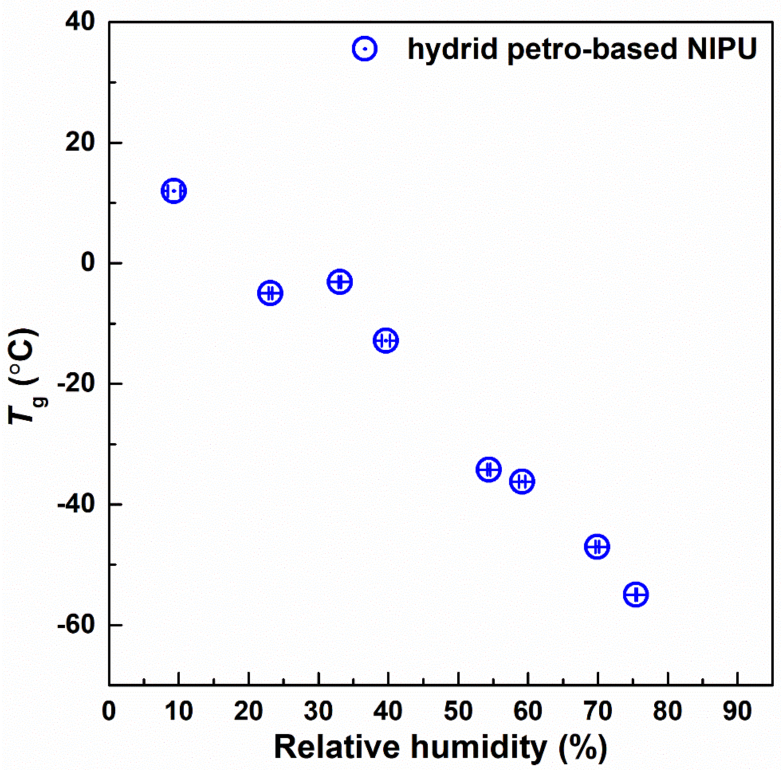


Figure S40. Glass transition temperatures of hybrid petro-based NIPU films at 10%, 20%, 40%, 60%, 70%, 75%, 80% and 85% RH

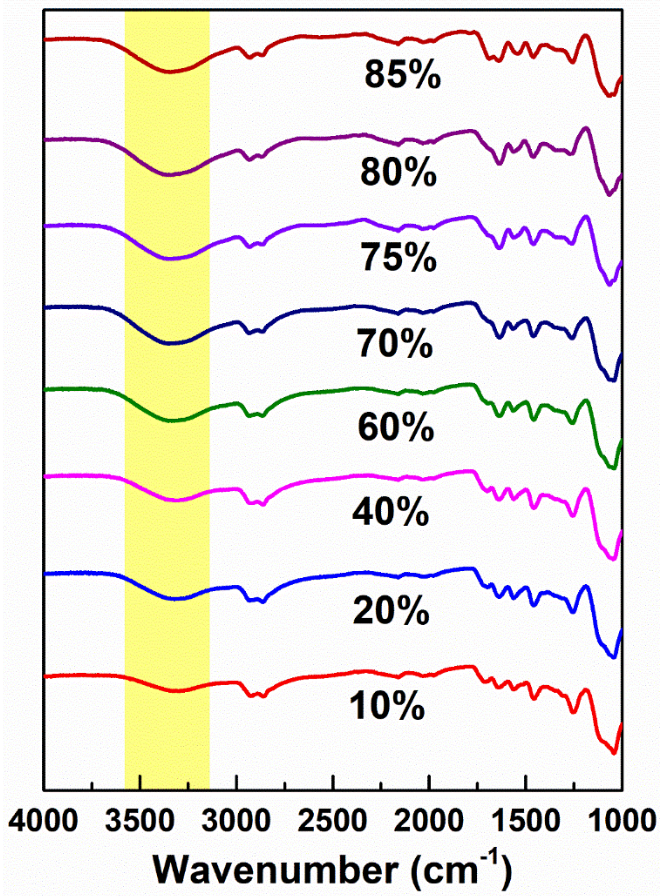


Figure S41. ATR-infrared spectra of hybrid petro-based NIPU films at 10%, 20%, 40%, 60%, 70%, 75%, 80% and 85% RH

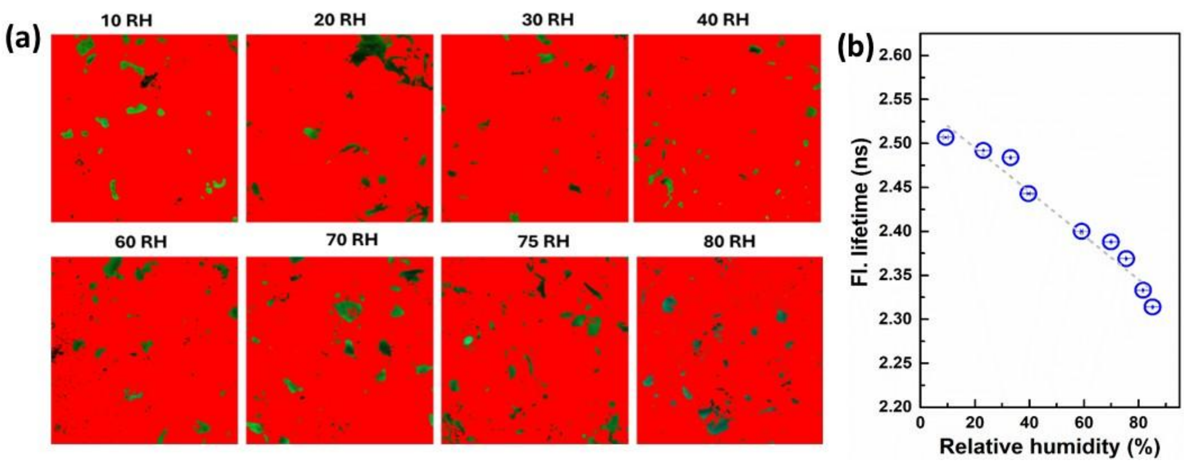
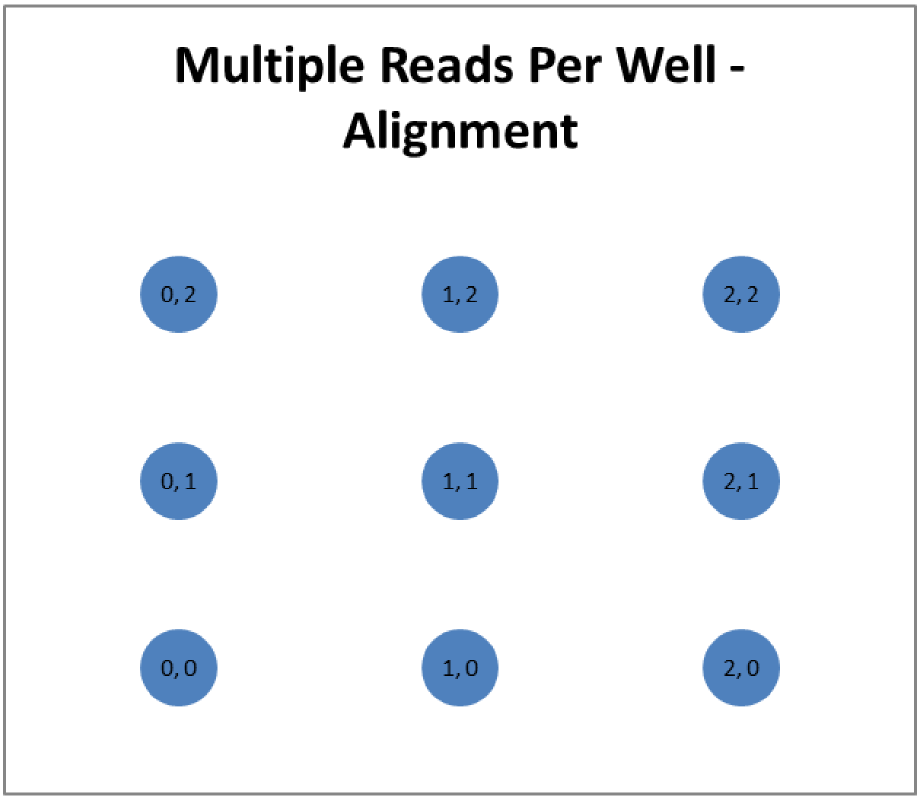


Figure S42. Fluorescence lifetime imaging microscopy (FLIM) images of hybrid petro-based NIPU film at different humidities (10-85%) acquired using leaser source of 440 nm, width × height = 1024 pixels × 1024 pixels

12. Humidity sensing by hybrid bio-based (90wt%) NIPU film

Fluorescence measurement for humidity sensing study by 90% hybrid bio-based NIPU film

The fluorescence of water absorbed hybrid bio-based NIPU films taking from different humidity chambers (10-85%) were recorded at 484 nm by the spectrofluorometer (Tecan Infinite 200Pro) at using 420 nm of excitation wavelength (λ_{ex}). The UV-star® microplate, 96 well, half area, μclear®, transparent, 10 ST/BTL of Greiner Bio-One GmbH, Germany (REF: 675801) was used as sample holder. The fluorescence intensities were recorded from the bottom of the well with manual gain of 60, number of flashes of 10, integration time of 20 μs, 0 μs of lag time. The excitation and emission slit widths were 10 and 20 nm for source and detector, respectively. From each well, nine times fluorescence intensities were measured (as shown below) from different portions of introduced 90% hybrid bio-based NIPU film. All the results were done twice with three replicates.



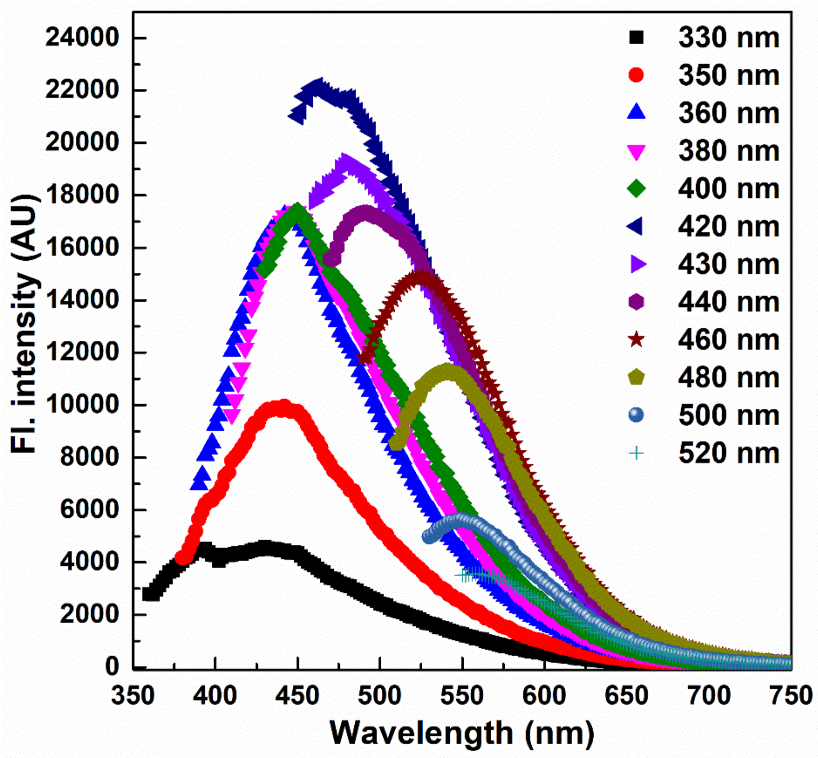


Figure S43. Excitation-dependent emission of hybrid bio-based NIPU film within 330-520 nm

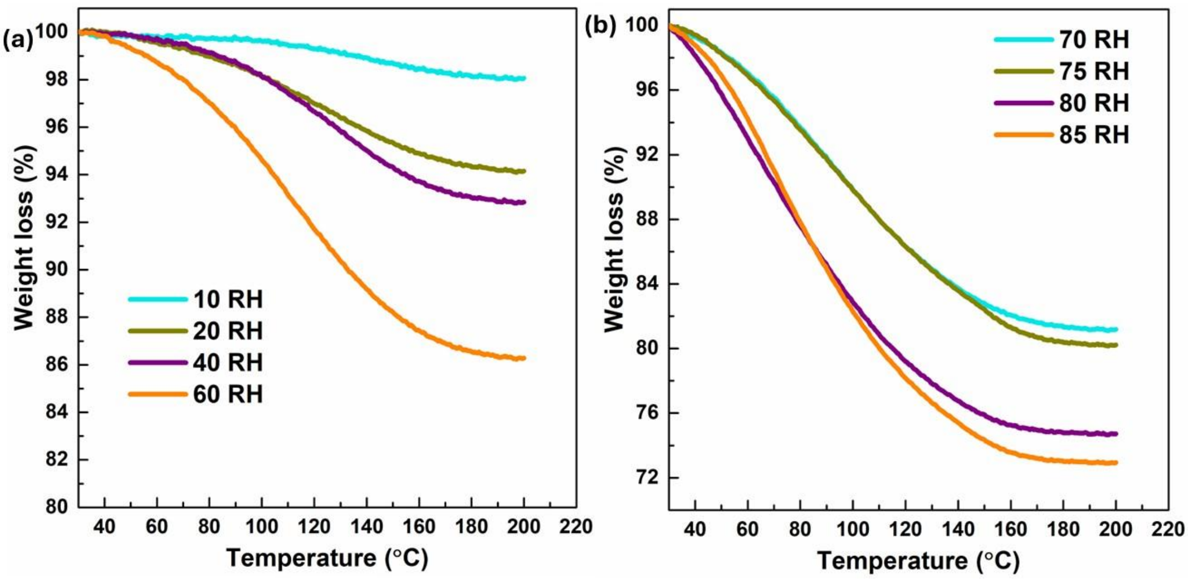


Figure S44. TGA thermograms of hybrid bio-based NIPU films at (a) 10%, 20%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

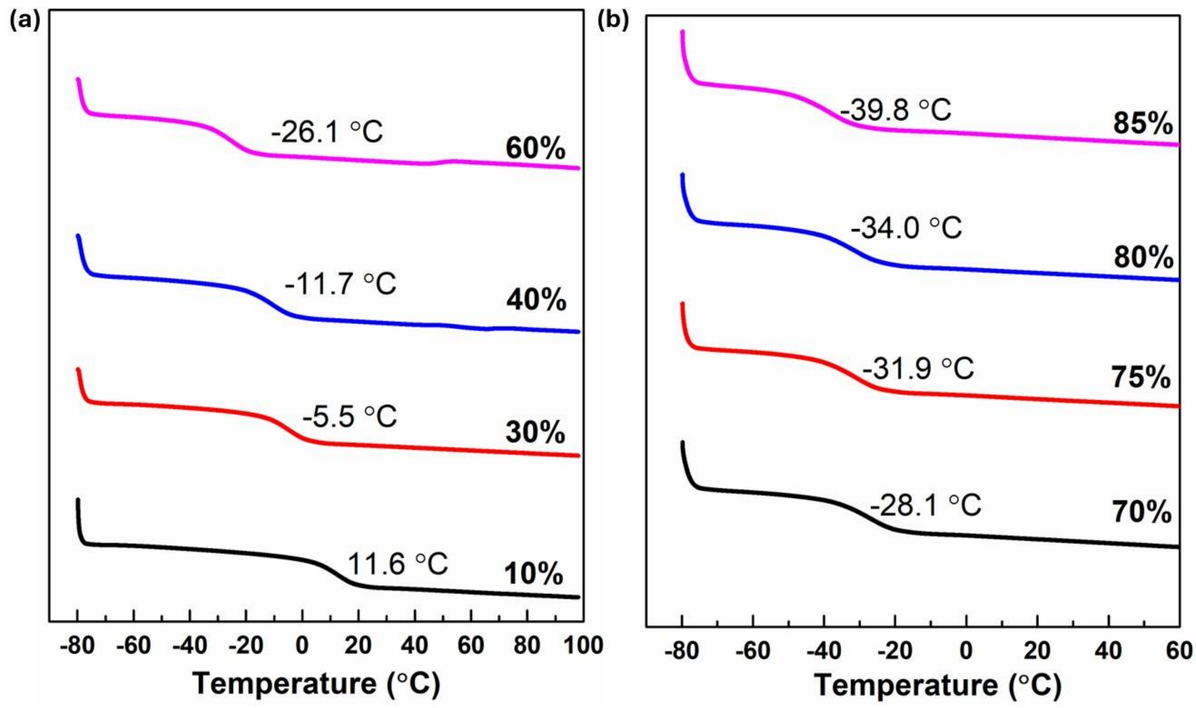


Figure S45. DSC thermograms of 90% hybrid bio-based NIPU film at (a) 10%, 30%, 40% and 60% RH and (b) 70%, 75%, 80% and 85% RH

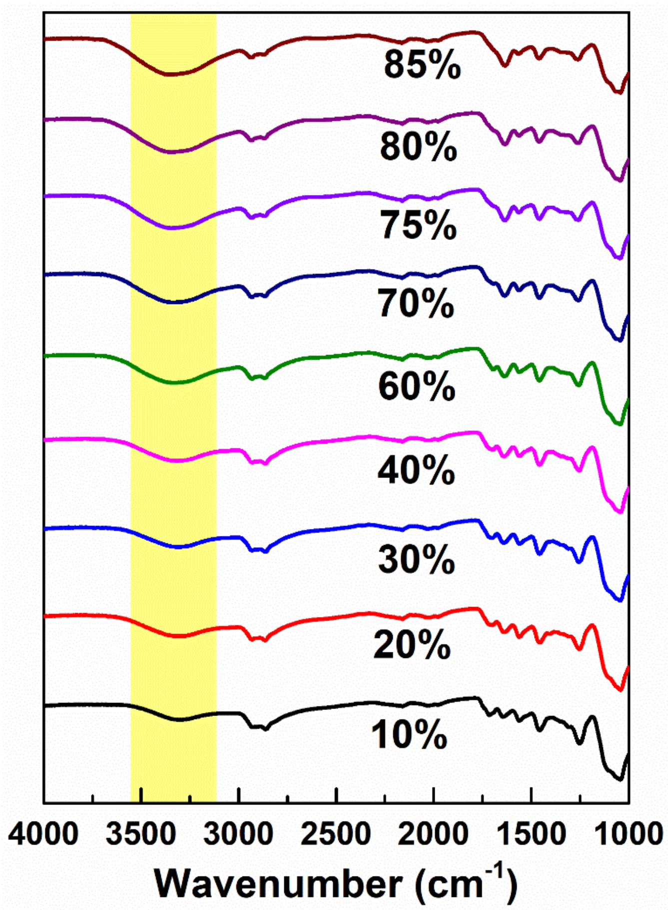


Figure S46. ATR-infrared spectra of hybrid bio-based NIPU films at 10%, 20%, 30%, 40%, 60%, 70%, 75%, 80% and 85% RH

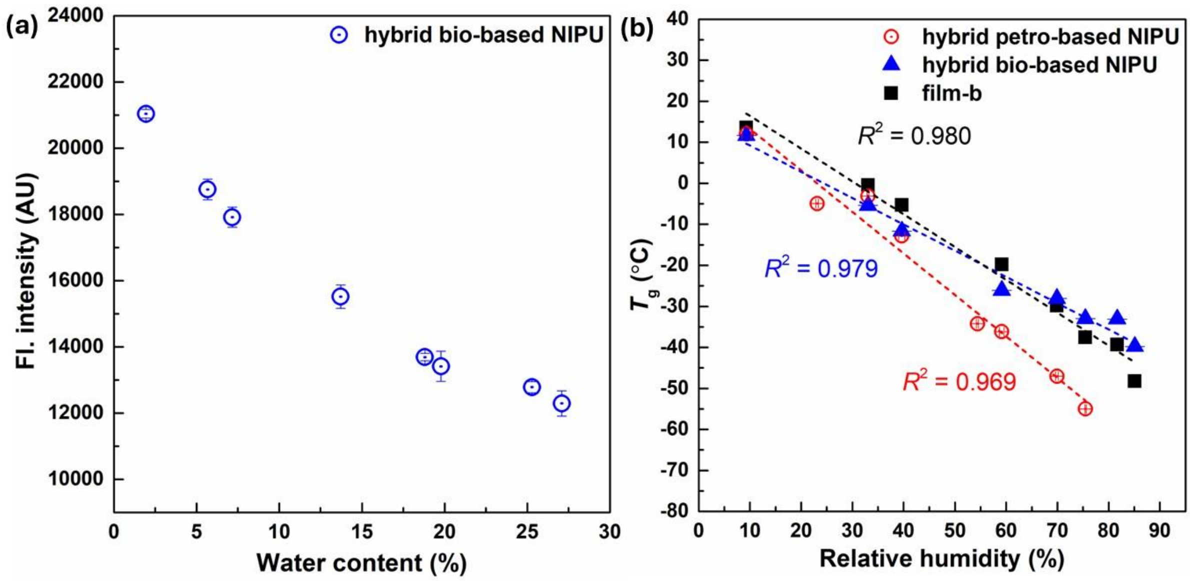


Figure S47. (a) Fluorescence intensities of hybrid bio-based NIPU films at different water content; (b) glass transition temperatures of hybrid petro-based NIPU film, hybrid bio-based NIPU film and film-b at RH (10-85%)

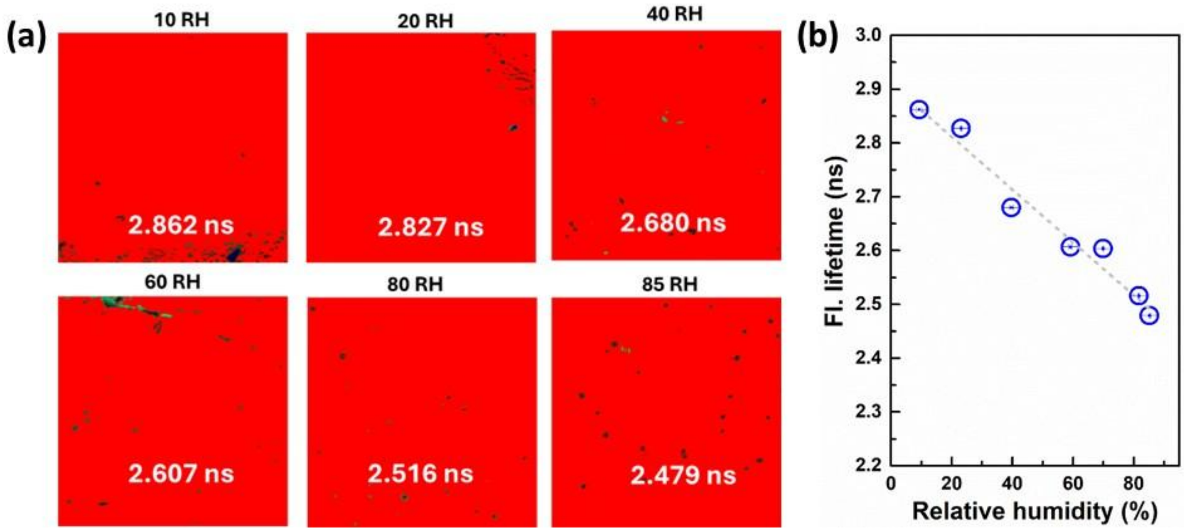


Figure S48. Fluorescence lifetime imaging microscopy (FLIM) images of hybrid bio-based NIPU film at different humidities (10-85%) acquired using leaser source of 440 nm, width × height = 1024 pixels × 1024 pixels

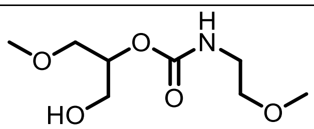
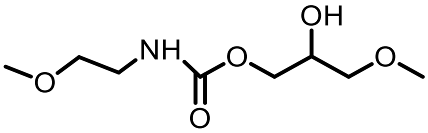
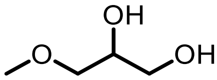
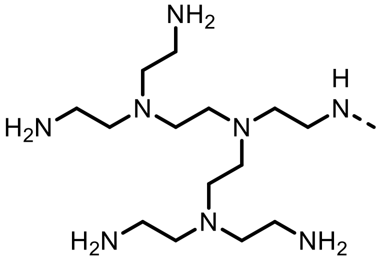
Table S6: Comparison of polyurethane-based humidity sensors

Name of system	***Origin of fluorescence***	***Nature of fluorescence sensing***	***Comments***	***References***
Metallosupramolecular (PU-Eu) elastomers	External fluorescent probe containing europium	Turn-off fluorescence	Fast and ultrasensitive humidity sensing	[1]
Polyurethane-based hybrid film	External fluorescent probe containing ruthenium-tris-bipyridyl complex	Turn-off fluorescence	Highly sensitive water sensor	[2]
Polyurethane-acrylate based adhesive films	Organic fluorescent sensors	Turn-off fluorescence	Less sensitive to water	[3]
Polyurethane-supported polyimide containing pyrene	External fluorescent probe containing pyrene unit	Not clear	Sensitive to humidity but needed more study	[4]
NIPU films from the reprocessing of NIPU foams (both at lower and higher temperature), a greener and safer alternative to classical isocyanate-based PU	Non-conventional fluorescence, i.e., fluorescence without any conjugated system and conventional emitting groups	Turn-off fluorescence	Sensitive to humidity; the fluorescence and lifetimes changes linearly; the hydroplasticization can be monitored easily; validated with different hybrid systems and upto 90% bio-based	This work

References:

[1] M. Li, Q. Lyu, L. Sun, B. Peng, L. Zhang, J. Zhu, *ACS Appl. Mater. Interfaces* **2020**, *12*, 39665.
[2] H.-S. Peng, X.-H. Li, F.-T. You, F. Teng, S.-H. Huang, *Microchim. Acta.* **2013**, *180*, 807.
[3] P. Bosch, A. Fernández, E. F. Salvador, T. Corrales, F. Catalina, C. Peinado, *Polymer* **2005**, *46*, 12200.
[4] C. Xu, L. Hao, X. Wang, X. Zhao, C. Wang, X. Zhu, *Appl. Surf. Sci.* **2025**, *702*, 163337.

13. Density functional theory calculation for humidity sensing

Structures of the model compounds used to make the aggregates		
 **Model compound-1**	 **Model compound-2**	 **Model compound-3**
 **PEI**		

Protocols to calculate the binding energy of water absorption

To investigate the mechanism of humidity sensing (water binding) and explore the interactions among chains and in between water molecules and chains, model NIPU film was created by making aggregation of model compounds: “1+2+3+PEI”. To validate the interactions of model compound with water molecules, aggregates of “1+2+3+PEI-water”, “1+2+3+PEI-two waters” and “1+2+3+PEI-three waters” were designed and optimized. All the model aggregates were computed theoretically via density functional theory (DFT) using B3LYP functional and 6-311+G(d,p) basis set. The energy levels of HOMOs/ LUMOs were calculated using GaussSum2.2. The orbitals were extracted using GaussView6.0.16.

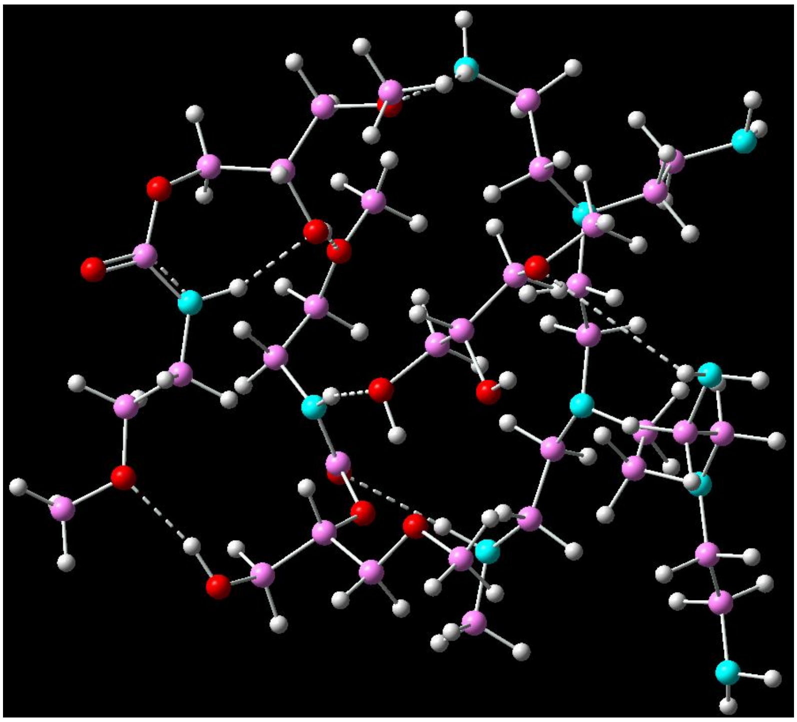


Figure S49. Optimized structure of aggregate representing the NIPU film showing intra molecular hydrogen bonding interactions

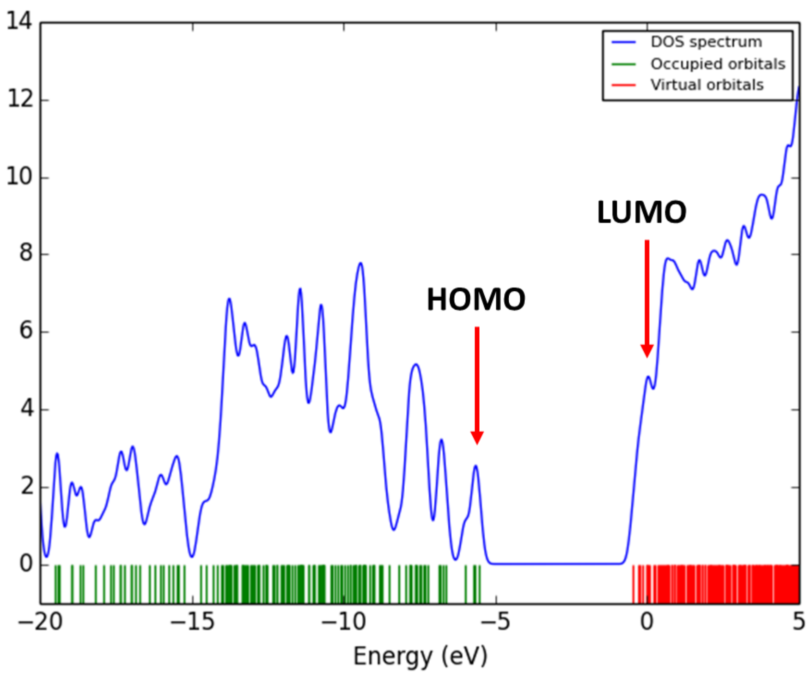


Figure S50. Density of state spectrum of aggregate representing the NIPU film using B3LYP/6-311+G(d,p)level in the range of -20 to 5 eV

Entry	MO levels	Energy (eV)
1	L+10	0.36
2	L+9	0.26
3	L+8	0.2
4	L+7	0.09
5	L+6	0.04
6	L+5	-0.01
7	L+4	-0.03
8	L+3	-0.16
9	L+2	-0.24
10	L+1	-0.31
11	LUMO	-0.46
12	HOMO	-5.53
13	H-1	-5.65
14	H-2	-5.71
15	H-3	-6
16	H-4	-6.62
17	H-5	-6.73
18	H-6	-6.83
19	H-7	-6.85
20	H-8	-7.23
21	H-9	-7.31
22	H-10	-7.35

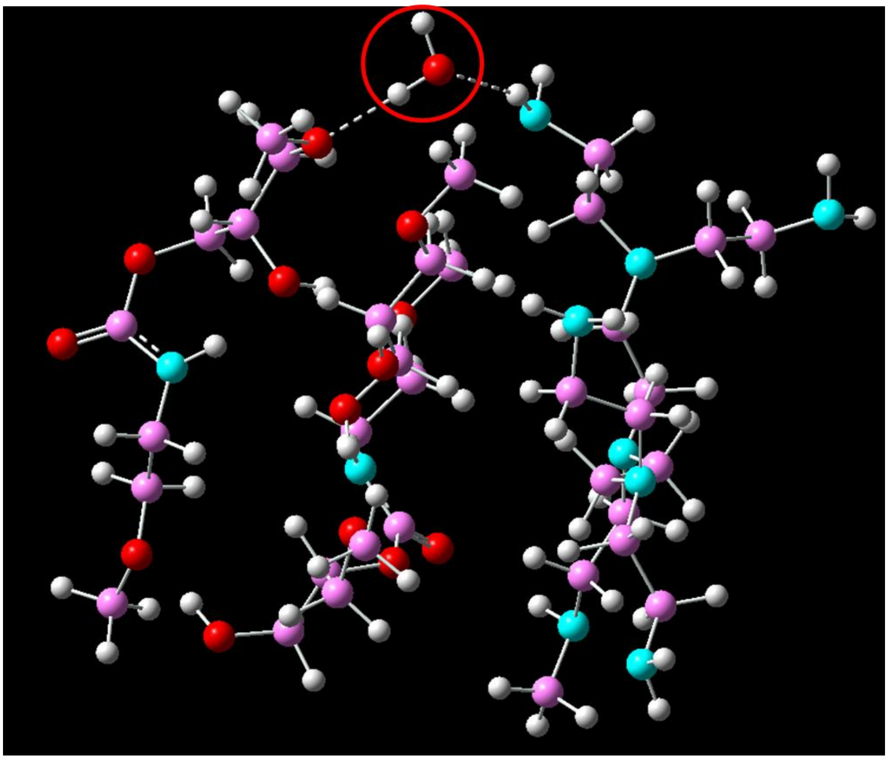


Figure S51. Optimized structure of aggregate with one water molecule showing intra molecular hydrogen bonding interactions and inter molecular hydrogen bonding with water molecule

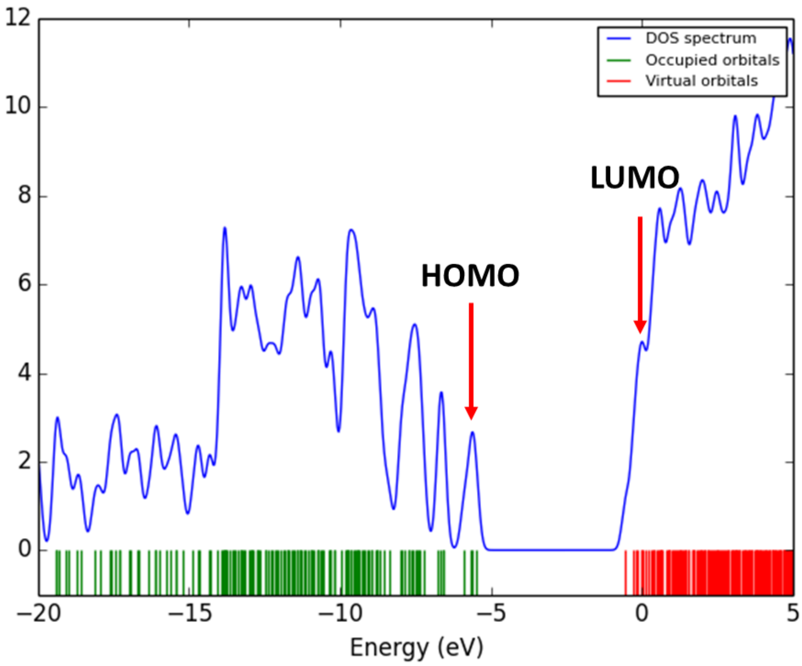


Figure S52. Density of state spectrum of aggregate with one water molecule using B3LYP/6-311+G(d,p) level in the range of -20 to 5 eV

Entry	MO levels	Energy (eV)
1	L+10	0.33
2	L+9	0.31
3	L+8	0.2
4	L+7	0.13
5	L+6	0.01
6	L+5	-0.01
7	L+4	-0.03
8	L+3	-0.16
9	L+2	-0.22
10	L+1	-0.3
11	LUMO	-0.54
12	HOMO	-5.49
13	H-1	-5.62
14	H-2	-5.66
15	H-3	-5.88
16	H-4	-6.59
17	H-5	-6.6
18	H-6	-6.66
19	H-7	-6.75
20	H-8	-7.23
21	H-9	-7.35
22	H-10	-7.4

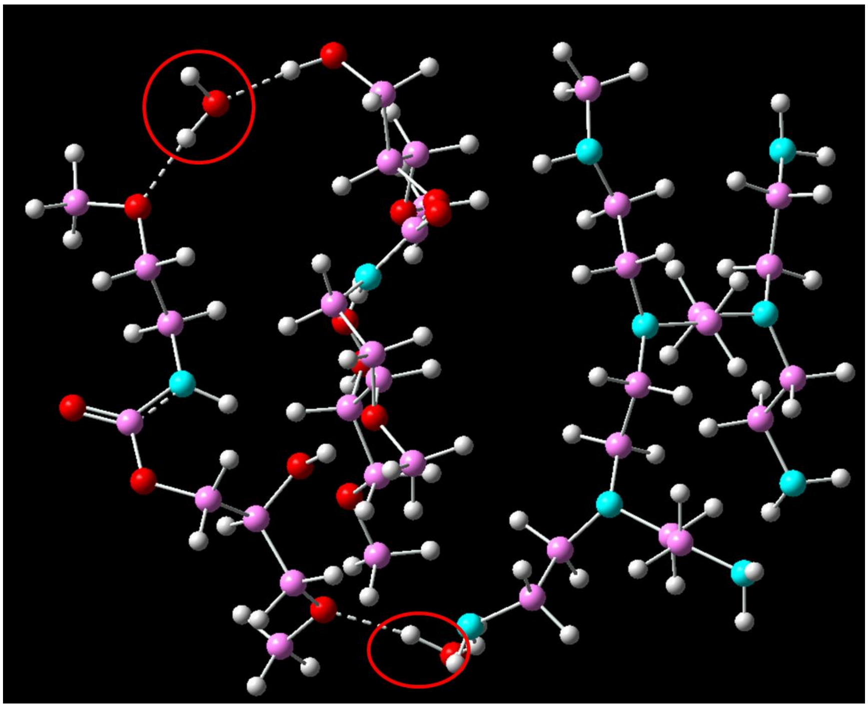


Figure S53. Optimized structure of aggregate with two water molecules showing intra molecular hydrogen bonding interactions and inter molecular hydrogen bonding with two water molecules

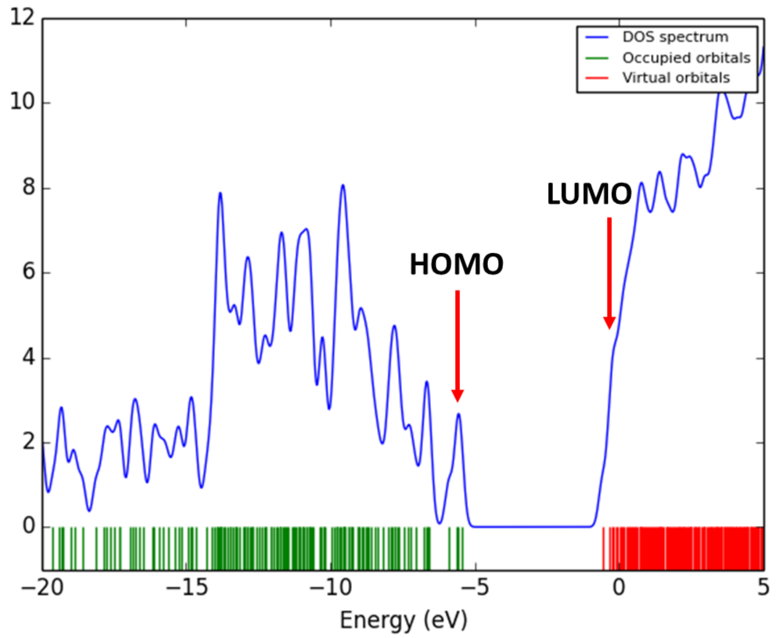


Figure S54. Density of state spectrum of aggregate with two water molecules using B3LYP/6-311+G(d,p) level in the range of -20 to 5 eV

Entry	MO levels	Energy (eV)
1	L+10	0.26
2	L+9	0.18
3	L+8	0.14
4	L+7	0.07
5	L+6	0.05
6	L+5	-0.08
7	L+4	-0.12
8	L+3	-0.22
9	L+2	-0.27
10	L+1	-0.35
11	LUMO	-0.59
12	HOMO	-5.47
13	H-1	-5.56
14	H-2	-5.62
15	H-3	-5.9
16	H-4	-6.56
17	H-5	-6.62
18	H-6	-6.7
19	H-7	-6.76
20	H-8	-7.03
21	H-9	-7.22
22	H-10	-7.29

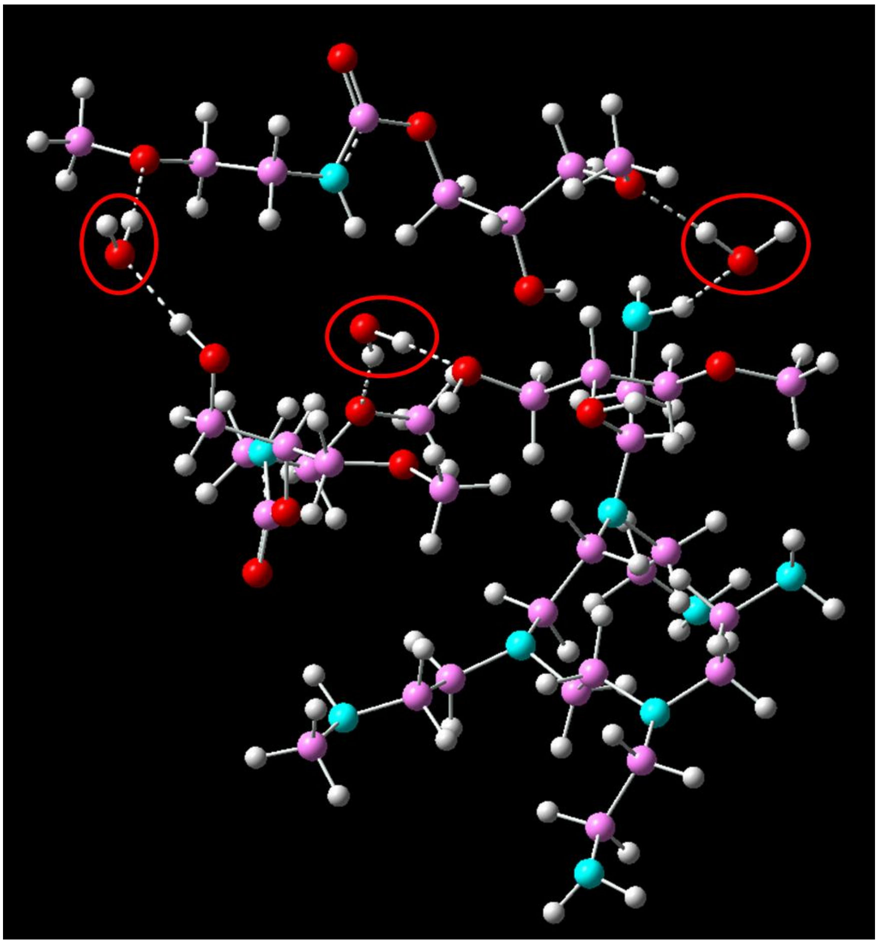


Figure S55. Optimized structure of aggregate with three water molecules showing intra molecular hydrogen bonding interactions and inter molecular hydrogen bonding with three water molecules

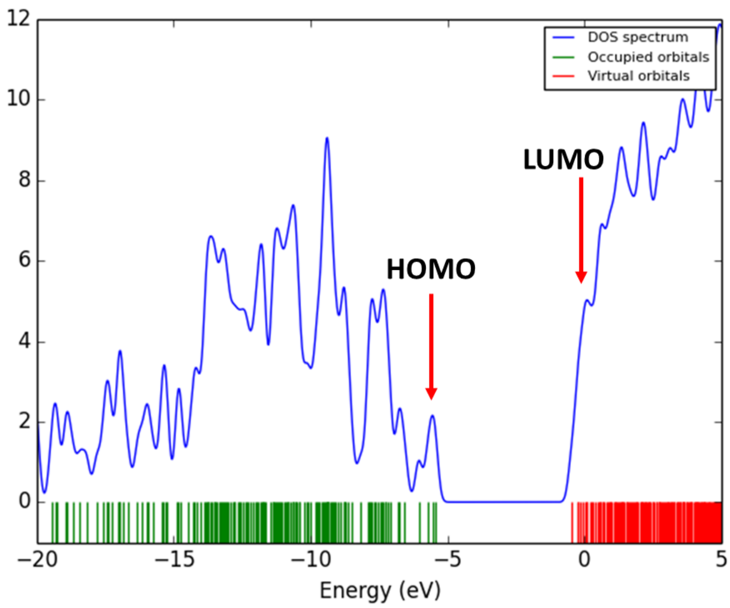


Figure S56. Density of state spectrum of aggregate with three water molecules using B3LYP/6-311+G(d,p) level in the range of -20 to 5 eV

Entry	MO levels	Energy (eV)
1	L+10	0.3
2	L+9	0.25
3	L+8	0.23
4	L+7	0.09
5	L+6	0.08
6	L+5	0.02
7	L+4	-0.05
8	L+3	-0.13
9	L+2	-0.23
10	L+1	-0.27
11	LUMO	-0.47
12	HOMO	-5.45
13	H-1	-5.56
14	H-2	-5.72
15	H-3	-6.06
16	H-4	-6.57
17	H-5	-6.75
18	H-6	-6.8
19	H-7	-7.09
20	H-8	-7.16
21	H-9	-7.27
22	H-10	-7.28

14. Calculation of binding energy of water absorption

The water binding energy to the aggregates was calculated using the following equation:

$$\boldsymbol{E_{wa} = E_{wf} - E_f - nE_w}$$

Were, the parameters represent:

E_{wa} = binding energy of water absorption

E_{wf} = energy of water absorbed film

E_f = energy of film

E_w = energy of single water molecule

n = number of water molecule

Here “aggregate is the model structure of “film”.

E_{wf} , E_f , and E_w were calculated from the DFT optimization [B3LYP/6-311+G(d,p)] of “water-absorbed-aggregate”, “aggregate” and “only water”, respectively.

Calculated parameters:

Energy of aggregate (Hartree): –2910.491990 Hartree

Energy of "aggregate with one water molecule": –2986.962539 Hartree

Energy of "aggregate with two water molecules": –3063.434597 Hartree

Energy of "aggregate with three water molecules": –3139.931567 Hartree

Energy of only water (Hartree): –76.458464 Hartree

Table S7: Binding energy of water absorption

Binding energy of single water absorption (Hartree; kcal/mol)	Binding energy of two water absorption (Hartree; kcal/mol)	Binding energy of three water absorption (Hartree; kcal/mol)
$E_{wa} = E_{wf} - E_f - E_w$	$E_{wa} = E_{wf} - E_f - 2E_w$	$E_{wa} = E_{wf} - E_f - 3E_w$
-0.012085; -7.583	-0.025679; -16.114	-0.064185; -40.277

15. Co-ordinates of all aggregates and computed structures

Co-ordinates of aggregate

Symbolic Z-matrix:

Charge = 0

Multiplicity = 1

C	-6.87358	-3.87139	-0.37416
O	-5.77176	-3.10919	0.20357
C	-5.82625	-1.67324	-0.07678
C	-5.00343	-0.94037	0.98215
N	-4.92194	0.49966	0.69693
O	-5.87348	2.66432	0.6955
C	-6.01749	1.28423	0.90912
O	-7.11773	0.86805	1.29202
H	-6.68876	-4.91065	-0.12024
H	-7.82455	-3.54429	0.05055
H	-6.89735	-3.75945	-1.46133
H	-5.43027	-1.4846	-1.07882
H	-6.86245	-1.33585	-0.02792
H	-5.46441	-1.10255	1.95658
H	-3.98434	-1.31762	1.01592
H	-3.99825	0.91213	0.56005
C	-4.82704	3.26786	-0.13617
H	-5.22384	4.26272	-0.32828
H	-4.74092	2.73315	-1.08423
C	-3.45895	3.33181	0.56165
H	-3.63859	3.24573	1.63305

O	-2.65249	2.16597	0.22706
H	-2.34184	2.14886	-0.7171
N	-2.07974	-1.28927	-1.61171
C	0.29228	-3.58479	2.93844
O	-0.52978	-3.21443	1.79705
C	-1.39076	-2.34208	-2.12948
O	-1.11812	-2.49034	-3.33468
O	-0.96162	-3.29993	-1.20605
C	-1.87176	-3.75701	-0.12767
C	-2.85971	-4.78356	-0.69102
O	-3.86083	-5.08706	0.30825
C	-1.02015	-4.32053	0.98633
H	0.52766	-2.64949	3.43539
H	-0.26214	-4.24664	3.60962
H	1.2069	-4.08097	2.6043
H	-2.44213	-2.91247	0.25214
H	-3.30901	-4.38353	-1.6045
H	-2.35485	-5.71553	-0.93613
H	-4.47523	-4.31987	0.40632
H	-1.63997	-4.97564	1.60345
H	-0.17878	-4.8815	0.57143
C	-2.80282	-0.38505	-2.5065
H	-3.59497	0.09677	-1.93385
H	-3.27633	-0.99481	-3.27761
C	-1.975	0.67699	-3.21844
H	-1.00139	0.2762	-3.50424
H	-2.50103	0.99768	-4.12448
O	-1.78979	1.86065	-2.3687
C	-1.05357	2.91651	-3.06743
H	-1.59569	3.20964	-3.97121
H	-0.96332	3.76873	-2.39766
H	-0.05769	2.56136	-3.34057
H	-1.94691	-1.05434	-0.61892
C	0.72424	1.98703	2.58725
C	-0.19869	0.77951	2.53514
C	-0.3016	0.17998	1.14787
O	-1.36053	-0.81319	1.067
O	0.32528	-0.24882	3.44157
H	1.72498	1.71804	2.23554
H	-1.19844	1.0712	2.86562
H	-0.56434	0.96188	0.44224
H	0.65195	-0.27122	0.86168
H	-1.0621	-1.66429	1.48711
H	0.49819	0.1929	4.29476
H	0.32958	2.80811	1.98212
O	0.79132	2.38191	3.99297
C	1.886	3.29354	4.29717
H	1.80212	4.21442	3.71181
H	1.79569	3.53146	5.35411
H	2.84851	2.81437	4.10143
N	5.9324	4.86383	-2.90012
C	4.59489	4.26282	-2.95885
C	4.16834	3.78008	-1.56365
N	2.83632	3.14118	-1.53808
C	2.83771	1.72474	-1.12156

C	3.31106	0.7773	-2.23368
N	3.26264	-0.63082	-1.80174
C	2.90206	-1.58909	-2.86623
C	2.42957	-2.95094	-2.33945
N	1.83471	-3.72885	-3.43404
C	1.72586	-5.16909	-3.18465
C	1.76326	3.95064	-0.94343
C	1.39072	5.18651	-1.77363
N	0.05994	5.67194	-1.36785
C	4.38018	-1.03925	-0.9254
C	3.91577	-1.57871	0.44478
N	5.02315	-1.70982	1.40645
C	5.13276	-0.63402	2.39853
C	5.37441	-3.0652	1.8447
C	6.06628	-3.88467	0.74406
N	6.41492	-5.21973	1.24403
C	4.11952	-0.70391	3.55938
N	4.22997	0.49783	4.407
H	6.44488	4.85558	-3.76962
H	5.97188	5.76839	-2.45038
H	4.63499	3.39812	-3.62236
H	3.82415	4.93444	-3.36202
H	4.18839	4.63035	-0.86598
H	4.92833	3.07824	-1.21202
H	3.44998	1.57403	-0.21753
H	1.81836	1.43585	-0.86872
H	2.64177	0.90676	-3.08443
H	4.31976	1.06521	-2.57328
H	2.0808	-1.15096	-3.43677
H	3.73105	-1.75946	-3.57291
H	3.28263	-3.51629	-1.95217
H	1.73508	-2.79356	-1.50128
H	0.93155	-3.34143	-3.69707
H	1.23913	-5.64465	-4.03687
H	2.72294	-5.60623	-3.08682
H	1.15165	-5.42544	-2.27927
H	2.01341	4.27465	0.08433
H	0.87419	3.3254	-0.87046
H	1.36604	4.89106	-2.82477
H	2.17286	5.95231	-1.67139
H	-0.16233	5.56251	-0.38227
H	-0.16426	6.5986	-1.70447
H	5.02727	-0.17801	-0.73869
H	5.00968	-1.78939	-1.42185
H	3.41925	-2.54372	0.31822
H	3.15057	-0.89559	0.82694
H	5.00509	0.32563	1.89385
H	6.15015	-0.63834	2.80575
H	4.50769	-3.64371	2.19875
H	6.06203	-2.97576	2.69114
H	6.92147	-3.30398	0.37086
H	5.37845	-4.01164	-0.09461
H	6.5051	-5.932	0.53436
H	7.19313	-5.23608	1.8894
H	4.27477	-1.64019	4.11549

H	3.10458	-0.73262	3.16047
H	3.48542	0.58425	5.0873
H	5.13526	0.60509	4.84976
C	-1.6773	5.0421	2.47221
H	-1.98421	4.13312	2.99123
H	-0.70723	5.35184	2.84909
H	-2.4092	5.83606	2.65032
C	-2.73161	4.65083	0.2856
H	-3.40866	5.48347	0.51506
H	-2.42115	4.72689	-0.75492
O	-1.5005	4.81609	1.04307

Co-ordinates of aggregate with one water molecule

Symbolic Z-matrix:

Charge = 0

Multiplicity = 1

C	-6.97858	-4.14581	-0.91285
O	-6.14378	-3.31378	-0.11369
C	-6.22709	-1.93232	-0.46297
C	-5.61413	-1.11432	0.67101
N	-5.5235	0.30533	0.33313
O	-6.47108	2.43952	0.24467
C	-6.63615	1.09028	0.44341
O	-7.74394	0.67638	0.69697
H	-6.82374	-5.17144	-0.57904
H	-8.03247	-3.87428	-0.78358
H	-6.71495	-4.06837	-1.97539
H	-5.68897	-1.75044	-1.40339
H	-7.27459	-1.64338	-0.5982
H	-6.21233	-1.25251	1.57484
H	-4.60088	-1.46507	0.8742
H	-4.60124	0.73157	0.39133
C	-5.28893	3.02606	-0.31903
H	-5.61652	4.02883	-0.60018
H	-4.99729	2.49537	-1.23104
C	-4.09447	3.09515	0.65363
H	-4.50299	2.97422	1.6603

O	-3.19559	2.00358	0.48713
H	-2.75555	2.03549	-0.38514
N	-2.16854	-1.32734	-1.48771
C	0.34913	-3.58097	3.04807
O	-0.45074	-3.15599	1.95103
C	-1.43517	-2.38906	-1.92769
O	-1.14913	-2.60163	-3.09008
O	-1.00158	-3.24582	-0.95206
C	-1.90177	-3.66186	0.10517
C	-2.88458	-4.70848	-0.44458
O	-3.90634	-4.99777	0.49269
C	-1.06118	-4.22209	1.23366
H	0.7363	-2.67768	3.51655
H	-0.25101	-4.14644	3.77231
H	1.18045	-4.20823	2.70408
H	-2.47006	-2.80916	0.48079
H	-3.29662	-4.34264	-1.39241
H	-2.35276	-5.64012	-0.65764
H	-4.61744	-4.34156	0.39428
H	-1.71698	-4.79705	1.89922
H	-0.29293	-4.89145	0.82394
C	-2.81256	-0.44365	-2.44809
H	-3.72183	-0.04265	-1.99178
H	-3.1118	-1.0552	-3.30136
C	-1.97388	0.7053	-2.98891
H	-0.97701	0.34875	-3.27167
H	-2.46207	1.10485	-3.88955
O	-1.85538	1.75685	-2.02382
C	-1.1137	2.86323	-2.54077
H	-1.63534	3.31198	-3.39567
H	-1.00249	3.60973	-1.75649
H	-0.11757	2.54334	-2.86411
H	-2.00727	-1.00962	-0.52893
C	0.9707	2.13383	2.55988
C	0.02726	0.93952	2.60827
C	-0.22098	0.36143	1.22353
O	-1.25593	-0.61665	1.21725
O	0.58131	-0.09199	3.43296
H	1.93114	1.83954	2.1132
H	-0.93571	1.26092	3.02621
H	-0.54487	1.16311	0.55769
H	0.71061	-0.06452	0.83069
H	-0.91339	-1.43889	1.61814
H	0.83574	0.33244	4.26158
H	0.53746	2.94548	1.96035
O	1.17573	2.56521	3.9008
C	2.16789	3.57883	4.01141
H	1.89241	4.46375	3.42425
H	2.22851	3.85108	5.06603
H	3.14514	3.21052	3.67472
N	6.38052	4.17922	-3.64115
C	4.98643	3.7253	-3.56232
C	4.63926	3.36146	-2.11422
N	3.26254	2.87677	-1.9445
C	3.18241	1.54099	-1.34553

C	3.49432	0.42936	-2.35521
N	3.36	-0.90292	-1.76096
C	2.975	-1.91268	-2.75331
C	2.52184	-3.24617	-2.15074
N	1.88986	-4.06634	-3.18118
C	1.66463	-5.445	-2.76337
C	2.36394	3.84072	-1.31104
C	2.03316	5.04985	-2.19164
N	0.8211	5.71299	-1.68965
C	4.51735	-1.28231	-0.93689
C	4.13168	-1.79289	0.46374
N	5.30689	-1.94609	1.32834
C	5.5932	-0.77608	2.15376
C	5.42169	-3.2308	2.01252
C	5.86414	-4.35659	1.07181
N	5.93949	-5.6269	1.80481
C	4.66887	-0.54927	3.36415
N	4.9983	0.7335	4.00526
H	6.68014	4.27804	-4.60467
H	6.49672	5.08493	-3.19719
H	4.88376	2.82931	-4.18037
H	4.25926	4.4576	-3.94087
H	4.8144	4.23752	-1.46946
H	5.35027	2.59821	-1.78374
H	3.83641	1.45093	-0.46101
H	2.1612	1.37722	-0.99559
H	2.77581	0.52218	-3.17293
H	4.49412	0.58143	-2.79898
H	2.13558	-1.50697	-3.32547
H	3.7866	-2.11253	-3.47592
H	3.38781	-3.79961	-1.76972
H	1.8559	-3.05307	-1.29408
H	0.99494	-3.64869	-3.4258
H	1.12132	-5.97819	-3.54716
H	2.62564	-5.9507	-2.62256
H	1.09086	-5.53911	-1.82534
H	2.75892	4.19722	-0.34046
H	1.42275	3.3313	-1.09834
H	1.83832	4.69146	-3.20718
H	2.90392	5.72161	-2.24751
H	0.89424	5.94726	-0.70067
H	0.65677	6.58016	-2.19016
H	5.16639	-0.41159	-0.80626
H	5.1336	-2.04018	-1.4432
H	3.61665	-2.75171	0.37943
H	3.39786	-1.09723	0.89168
H	5.55167	0.11621	1.52199
H	6.62976	-0.85042	2.50856
H	4.49056	-3.54273	2.51339
H	6.17825	-3.12573	2.79895
H	6.80648	-4.05719	0.59078
H	5.12448	-4.47877	0.27518
H	6.07325	-6.4067	1.17079
H	6.7249	-5.62922	2.44826
H	4.74617	-1.40727	4.04849

H	3.62776	-0.49826	3.03392
H	4.38277	0.90974	4.79254
H	5.94552	0.71777	4.37289
C	-2.55875	4.42122	2.83444
H	-2.80847	3.38498	3.07683
H	-1.65471	4.69727	3.37619
H	-3.38242	5.07972	3.13828
C	-3.38749	4.45599	0.57768
H	-4.12233	5.24202	0.80673
H	-2.99751	4.63582	-0.42817
O	-2.26657	4.57576	1.44545
O	0.15512	6.08134	1.33201
H	-0.0603	6.91816	1.75386
H	-0.68931	5.60087	1.25796

Co-ordinates of aggregate with two water molecules

Symbolic Z-matrix:

Charge = 0

Multiplicity = 1

C	-7.60558	-3.23887	0.0312
O	-6.3347	-3.03308	-0.5832
C	-6.09076	-1.69875	-1.03936
C	-5.65002	-0.77104	0.09859
N	-5.3618	0.57442	-0.39988
O	-6.07914	2.72083	-0.98448
C	-6.39812	1.43491	-0.63065
O	-7.56713	1.13105	-0.54991
H	-7.67545	-4.30182	0.2625
H	-7.70354	-2.66669	0.95847
H	-8.41664	-2.95737	-0.65021
H	-5.29429	-1.77862	-1.78213
H	-6.9866	-1.29899	-1.52579
H	-6.43013	-0.71721	0.86201
H	-4.7377	-1.15408	0.55918
H	-4.43195	0.94132	-0.21304
C	-4.74825	3.14449	-1.32058
H	-4.90778	4.10967	-1.80327
H	-4.30819	2.46499	-2.05658
C	-3.81535	3.28305	-0.09802
H	-4.4551	3.26396	0.7884

O	-2.95518	2.15041	0.04267
H	-2.39369	2.04285	-0.75182
N	-1.59521	-1.46336	-1.52439
C	-0.65358	-3.91323	3.40367
O	-1.04774	-3.5461	2.08543
C	-0.65307	-2.38589	-1.83602
O	-0.14201	-2.50817	-2.93428
O	-0.27313	-3.18202	-0.78158
C	-1.25243	-4.11567	-0.25307
C	-1.39361	-5.31672	-1.20489
O	-2.42339	-6.18992	-0.78224
C	-0.78415	-4.55762	1.11633
H	-0.91134	-3.0776	4.05168
H	-1.18524	-4.81614	3.72969
H	0.42666	-4.09992	3.44716
H	-2.22373	-3.61926	-0.16113
H	-1.56678	-4.94666	-2.22122
H	-0.45897	-5.88459	-1.21667
H	-3.27743	-5.81516	-1.06273
H	-1.32272	-5.47461	1.38218
H	0.29234	-4.77201	1.08176
C	-2.23287	-0.67512	-2.56836
H	-3.17382	-0.28759	-2.17144
H	-2.47574	-1.34218	-3.40049
C	-1.40984	0.46836	-3.14583
H	-0.39027	0.12601	-3.34914
H	-1.8616	0.78	-4.09878
O	-1.3747	1.59563	-2.26266
C	-0.55578	2.64166	-2.78872
H	-0.94936	2.99019	-3.75256
H	-0.55247	3.46986	-2.08028
H	0.47216	2.29195	-2.93275
H	-1.82859	-1.30783	-0.54189
C	-1.53686	1.52354	3.9846
C	-2.1095	0.24537	3.38418
C	-1.47332	-0.07323	2.03897
O	-2.15326	-1.12054	1.34843
O	-1.88576	-0.85561	4.26653
H	-0.44624	1.43076	4.09899
H	-3.18923	0.3812	3.23468
H	-1.53352	0.81335	1.40705
H	-0.41942	-0.33818	2.1867
H	-1.85242	-1.97606	1.71506
H	-2.19292	-0.57919	5.13878
H	-1.75398	2.38259	3.3344
O	-2.14244	1.69619	5.25997
C	-1.58888	2.76103	6.0115
H	-1.71495	3.72252	5.49571
H	-2.12083	2.79589	6.96242
H	-0.51923	2.60061	6.20251
N	6.23946	4.95944	-3.42861
C	4.92571	4.31568	-3.30803
C	4.68978	3.88576	-1.85553
N	3.40515	3.2036	-1.64395
C	3.54523	1.86491	-1.05987

C	3.94661	0.81985	-2.10868
N	4.04809	-0.52358	-1.53854
C	3.7111	-1.57234	-2.50693
C	3.44553	-2.94158	-1.87495
N	2.88647	-3.84626	-2.87489
C	2.81886	-5.23094	-2.42698
C	2.39691	4.02107	-0.97312
C	1.88825	5.19108	-1.82164
N	0.61748	5.69206	-1.27364
C	5.30738	-0.76058	-0.81818
C	5.09186	-1.20518	0.63914
N	6.35797	-1.3968	1.35214
C	6.93092	-0.17502	1.91102
C	6.39465	-2.55478	2.24329
C	6.58399	-3.8729	1.48427
N	6.60163	-4.99946	2.4263
C	6.23903	0.40975	3.15693
N	6.91347	1.65458	3.54874
H	6.48216	5.11958	-4.39985
H	6.25007	5.86216	-2.96403
H	4.92395	3.423	-3.93928
H	4.09054	4.94562	-3.646
H	4.76336	4.76823	-1.19991
H	5.51472	3.22816	-1.5663
H	4.26081	1.86041	-0.21996
H	2.58098	1.55688	-0.64981
H	3.16991	0.81695	-2.87686
H	4.88164	1.12386	-2.61173
H	2.79622	-1.26547	-3.02111
H	4.49106	-1.68916	-3.28044
H	4.38382	-3.37895	-1.51427
H	2.78692	-2.81508	-0.99915
H	1.95058	-3.52576	-3.11352
H	2.31773	-5.8363	-3.18619
H	3.83086	-5.62989	-2.30043
H	2.2824	-5.36709	-1.47122
H	2.76231	4.41352	-0.00388
H	1.53958	3.38212	-0.75129
H	1.71302	4.82799	-2.83923
H	2.66323	5.96937	-1.88672
H	0.69889	5.88507	-0.27548
H	0.36135	6.56521	-1.72352
H	5.90548	0.15658	-0.82264
H	5.91624	-1.51755	-1.33075
H	4.54086	-2.14683	0.64137
H	4.43539	-0.47408	1.13521
H	6.94485	0.59808	1.13817
H	7.98182	-0.37528	2.1575
H	5.49825	-2.64338	2.87817
H	7.2452	-2.42905	2.92324
H	7.48881	-3.78929	0.86522
H	5.7437	-4.02704	0.80148
H	6.55602	-5.88584	1.93629
H	7.45826	-5.00471	2.97126
H	6.21725	-0.34665	3.95578

H	5.19951	0.65541	2.92148
H	6.442	2.09791	4.3297
H	7.86799	1.47147	3.84352
C	-3.36438	5.45576	2.13695
H	-4.16236	4.75966	2.41712
H	-2.78055	5.70113	3.02367
H	-3.81103	6.37396	1.73689
C	-3.03463	4.60414	-0.08156
H	-3.69989	5.43011	-0.36668
H	-2.19918	4.57891	-0.78611
O	-2.46196	4.88083	1.19549
O	0.17236	5.66691	1.81078
H	0.62762	4.95382	2.26754
H	-0.69926	5.30772	1.5628
O	-4.74666	-4.95985	-1.76949
H	-5.25287	-5.3736	-2.47405
H	-5.34887	-4.32852	-1.32585

Co-ordinates of aggregate with three water molecules

Symbolic Z-matrix:

Charge = 0

Multiplicity = 1

C	8.90503	-2.52588	0.7437
O	7.85512	-2.07965	-0.10723
C	7.2082	-0.89945	0.37708
C	6.2492	-0.38424	-0.69402
N	5.51839	0.78516	-0.22355
O	5.39379	3.08161	0.20432
C	6.11059	2.0098	-0.26198
O	7.23273	2.21004	-0.67583
H	9.31914	-3.4324	0.30222
H	9.69115	-1.76595	0.81767
H	8.52881	-2.75514	1.74847
H	6.66055	-1.13041	1.30104
H	7.95934	-0.13261	0.59535
H	6.81434	-0.13302	-1.59355
H	5.51563	-1.15261	-0.94403
H	4.54072	0.629	0.01484
C	4.10883	2.97627	0.83414
H	4.10398	3.74958	1.608
H	3.97182	2.01268	1.32577
C	2.95469	3.21656	-0.15302

H	3.03201	2.47333	-0.95372
O	1.7223	2.97347	0.50378
H	1.35443	3.78509	0.93623
N	2.19213	-2.91967	1.67666
C	-0.72269	-2.86583	-3.5379
O	0.16975	-2.71629	-2.43548
C	1.14926	-3.75412	1.39981
O	0.44182	-4.25498	2.25466
O	0.90807	-4.04658	0.09532
C	1.82041	-3.72688	-0.98308
C	3.00629	-4.70232	-0.98874
O	3.88265	-4.33798	-2.03989
C	1.02444	-3.84505	-2.26846
H	-1.27123	-1.93091	-3.63198
H	-0.16724	-3.05391	-4.46565
H	-1.41481	-3.69721	-3.35848
H	2.19084	-2.70287	-0.89352
H	3.50554	-4.66833	-0.01624
H	2.6285	-5.72322	-1.13477
H	4.80205	-4.30998	-1.71788
H	1.72465	-3.91175	-3.1087
H	0.42238	-4.76203	-2.2289
C	2.46655	-2.53944	3.05679
H	3.51547	-2.23805	3.11757
H	2.32697	-3.4194	3.6863
C	1.58905	-1.4197	3.59938
H	0.5293	-1.6791	3.49029
H	1.80275	-1.28322	4.66925
O	1.87164	-0.20709	2.90131
C	1.12815	0.90723	3.38717
H	1.40082	1.12781	4.42716
H	1.37628	1.75467	2.74964
H	0.0498	0.7202	3.33356
H	2.55384	-2.29874	0.95998
C	-1.48562	2.60241	-2.54663
C	-0.53305	1.44244	-2.80723
C	-0.11068	0.75908	-1.5157
O	0.98694	-0.13697	-1.70072
O	-1.15769	0.47525	-3.65616
H	-2.38212	2.24567	-2.01898
H	0.36652	1.83076	-3.30379
H	0.22929	1.51788	-0.80695
H	-0.96745	0.22684	-1.08668
H	0.66841	-0.99521	-2.0444
H	-1.53083	0.96723	-4.39836
H	-1.00002	3.37436	-1.93574
O	-1.8521	3.13276	-3.81558
C	-2.84594	4.14716	-3.72812
H	-2.49711	4.98307	-3.10874
H	-3.0253	4.50416	-4.74331
H	-3.77996	3.74936	-3.31253
N	-4.67403	3.96986	5.14532
C	-3.49358	3.28655	4.6042
C	-3.59878	3.19154	3.07825
N	-2.4563	2.50215	2.45801

C	-2.84769	1.32657	1.6707
C	-3.24163	0.12374	2.53676
N	-3.56997	-1.04227	1.71359
C	-3.27227	-2.31214	2.38549
C	-3.24726	-3.52228	1.4464
N	-2.73553	-4.69344	2.14922
C	-2.88849	-5.92889	1.38929
C	-1.56893	3.38867	1.70402
C	-0.79224	4.37452	2.58003
N	0.25217	5.04271	1.77552
C	-4.91893	-0.9754	1.13209
C	-4.9421	-1.19712	-0.39234
N	-6.26825	-0.93634	-0.96425
C	-6.38168	0.33419	-1.67228
C	-6.91012	-2.07286	-1.6179
C	-7.41498	-3.11931	-0.61874
N	-8.06183	-4.2263	-1.33379
C	-5.69905	0.41087	-3.05003
N	-5.83466	1.77018	-3.59658
H	-4.70591	3.90485	6.15649
H	-4.6699	4.95688	4.90771
H	-3.4677	2.27375	5.01517
H	-2.53968	3.76268	4.87517
H	-3.70375	4.20415	2.65893
H	-4.53098	2.67135	2.83845
H	-3.66124	1.56733	0.96406
H	-1.99229	1.01643	1.0682
H	-2.38427	-0.12367	3.1672
H	-4.06668	0.38954	3.2208
H	-2.27959	-2.22309	2.83644
H	-3.97958	-2.52148	3.20773
H	-4.26385	-3.75463	1.10883
H	-2.6596	-3.26914	0.547
H	-1.74598	-4.55674	2.34464
H	-2.4167	-6.75009	1.93355
H	-3.95136	-6.16863	1.27822
H	-2.44314	-5.8894	0.38002
H	-2.11805	3.95674	0.92887
H	-0.83735	2.76875	1.18344
H	-0.30618	3.82024	3.38787
H	-1.4778	5.0951	3.046
H	-0.15327	5.54807	0.98491
H	0.73536	5.73256	2.34351
H	-5.35098	0.01088	1.32662
H	-5.59214	-1.6971	1.61776
H	-4.62821	-2.21792	-0.62705
H	-4.18393	-0.54363	-0.83903
H	-5.96928	1.12633	-1.03972
H	-7.44821	0.56551	-1.79379
H	-6.25795	-2.5801	-2.34769
H	-7.77219	-1.69331	-2.1789
H	-8.0623	-2.61716	0.11484
H	-6.5676	-3.53477	-0.06562
H	-8.23916	-5.0086	-0.71391
H	-8.95746	-3.93925	-1.71596

H	-6.11791	-0.36447	-3.7082
H	-4.631	0.1987	-2.94542
H	-5.37181	1.84201	-4.49693
H	-6.81318	1.99528	-3.75336
C	2.45074	4.36562	-3.06778
H	2.5384	3.27456	-3.05957
H	1.65329	4.64944	-3.75434
H	3.39823	4.7997	-3.40837
C	3.05337	4.62059	-0.75413
H	4.06723	4.78554	-1.13514
H	2.85679	5.36448	0.02381
O	2.09678	4.87722	-1.78546
O	-0.24989	6.16442	-1.01183
H	-0.28649	7.03548	-1.41688
H	0.55584	5.73801	-1.36568
O	6.56631	-4.24629	-1.29338
H	7.09485	-4.46767	-2.06611
H	6.97915	-3.44715	-0.90724
O	2.89632	-0.35128	0.27404
H	2.21503	-0.22774	-0.42468
H	2.45549	-0.15714	1.12182

Coordinates of small aggregate
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	2.64125	-5.84275	0.22966
O	2.47911	-4.41746	-0.02619
C	3.68661	-3.74689	-0.50697
C	3.25403	-2.40117	-1.08139
N	4.39517	-1.56869	-1.47925
O	6.09837	-0.94593	-2.98339
C	5.09522	-1.85712	-2.61283
O	4.89098	-2.83485	-3.34055
H	1.677	-6.19494	0.58318
H	2.91655	-6.36542	-0.68894
H	3.40197	-6.0166	0.99494
H	4.38798	-3.61207	0.32181
H	4.15523	-4.35173	-1.28516
H	2.60415	-2.57814	-1.93852
H	2.69014	-1.84371	-0.33607
H	4.4918	-0.6536	-1.05066
C	6.76915	-0.02349	-2.06181
H	7.69716	0.22157	-2.56728
H	6.98335	-0.5113	-1.10986
C	5.96688	1.25848	-1.8459
H	5.35886	1.476	-2.72456
O	5.03244	1.12427	-0.74422
H	5.48771	1.19753	0.15001

N	2.95243	-0.36786	2.89606
C	-2.59362	0.2265	3.39156
O	-1.26116	-0.18034	2.97718
C	2.62831	-1.25479	3.8704
O	3.42389	-1.90319	4.56328
O	1.23302	-1.40045	4.04465
C	0.46258	-1.89005	2.8762
C	0.72708	-3.38865	2.68908
O	0.21401	-3.82269	1.40505
C	-0.99185	-1.6066	3.15962
H	-2.65974	1.29598	3.21379
H	-3.35478	-0.28846	2.8006
H	-2.74618	0.01976	4.45394
H	0.77907	-1.35944	1.97838
H	1.80015	-3.57288	2.77171
H	0.2251	-3.95887	3.47112
H	0.95448	-3.89632	0.75874
H	-1.60971	-2.18125	2.46562
H	-1.22406	-1.89038	4.18987
C	4.30948	-0.24893	2.38537
H	4.28228	-0.3608	1.30267
H	4.90696	-1.05576	2.80291
C	4.94573	1.1032	2.70691
H	4.21482	1.91111	2.61956
H	5.37695	1.11727	3.70992
O	6.01235	1.30704	1.71606
C	6.96024	2.36844	2.02653
H	7.52454	2.11512	2.9256
H	7.62677	2.43468	1.17194
H	6.44456	3.32138	2.17051
H	2.23107	0.25388	2.51362
C	1.34491	3.2135	-1.01552
C	1.68464	2.41306	0.23204
C	0.43471	2.00916	0.99154
O	0.81349	1.38668	2.24722
O	2.40343	1.19413	-0.1211
H	0.8221	2.56974	-1.7295
H	2.31218	3.0282	0.88563
H	-0.16277	2.90467	1.18589
H	-0.15438	1.3202	0.38179
H	0.044	0.9045	2.64228
H	3.28321	1.39871	-0.51797
H	0.71381	4.07552	-0.77315
O	2.61003	3.67014	-1.59407
C	2.43708	4.35179	-2.86114
H	1.81879	5.24838	-2.74685
H	3.4292	4.64031	-3.19877
H	1.97599	3.69426	-3.60468
N	-1.49146	5.71004	-0.31648
C	-2.8713	5.25762	-0.56776
C	-3.12087	3.92674	0.15017
N	-4.49028	3.41912	-0.03044
C	-4.60751	1.95139	0.02816
C	-5.85119	1.41	-0.69341
N	-5.87969	-0.06329	-0.68675

C	-7.21369	-0.67914	-0.58262
C	-7.18261	-2.06396	0.07569
N	-8.54073	-2.60285	0.19662
C	-8.63613	-4.00108	0.62443
C	-5.52439	4.15901	0.72228
C	-6.54335	4.8766	-0.17616
N	-7.51777	5.60564	0.64546
C	-4.97963	-0.70365	-1.67175
C	-3.81782	-1.50294	-1.04482
N	-2.92063	-2.04994	-2.07108
C	-1.81768	-1.17976	-2.49649
C	-2.66766	-3.49796	-2.04425
C	-3.84699	-4.30674	-2.60733
N	-3.54746	-5.74268	-2.57484
C	-0.60495	-1.11531	-1.54537
N	0.37098	-0.13468	-2.0416
H	-1.15488	6.39936	-0.97519
H	-1.32346	6.00699	0.63698
H	-2.99413	5.09523	-1.6388
H	-3.62618	5.99541	-0.26299
H	-2.87077	4.04676	1.22161
H	-2.42247	3.19846	-0.25925
H	-3.72113	1.53037	-0.44649
H	-4.62966	1.5765	1.06569
H	-6.74825	1.76864	-0.18663
H	-5.86746	1.82207	-1.71409
H	-7.83697	-0.02244	0.03016
H	-7.70899	-0.77692	-1.56127
H	-6.60939	-2.7563	-0.54621
H	-6.65129	-1.98471	1.03872
H	-9.14361	-1.99521	0.74109
H	-9.68503	-4.29237	0.68537
H	-8.15947	-4.643	-0.11894
H	-8.16253	-4.21006	1.5981
H	-5.0607	4.91215	1.36555
H	-6.05772	3.47191	1.3945
H	-6.99382	4.14735	-0.86362
H	-6.00853	5.59851	-0.79478
H	-7.99542	6.358	0.17043
H	-8.16652	5.01614	1.15019
H	-4.55832	0.06368	-2.32969
H	-5.55028	-1.37747	-2.32002
H	-4.22419	-2.32332	-0.45065
H	-3.28217	-0.85398	-0.33889
H	-2.19516	-0.1637	-2.62844
H	-1.47744	-1.51116	-3.48388
H	-2.43367	-3.87382	-1.03966
H	-1.78812	-3.69411	-2.66415
H	-4.08242	-3.91361	-3.6072
H	-4.72858	-4.13649	-1.9841
H	-4.35239	-6.34861	-2.64334
H	-2.8105	-6.03004	-3.20513
H	-0.19197	-2.12617	-1.41667
H	-0.93831	-0.79	-0.55717
H	1.09675	0.13532	-1.38316

H	0.7589	-0.36722	-2.94785
C	7.38681	4.62141	-1.13706
H	8.31553	4.49958	-1.6543
H	7.04782	5.63047	-1.24557
H	7.52507	4.40127	-0.09912
C	6.89734	2.31354	-1.57708
H	7.72585	2.23407	-2.24951
H	7.23681	2.16338	-0.57353
O	6.33904	3.66129	-1.73032

Coordinates of medium aggregate

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	12.45747	-1.83996	-1.20452
O	11.00244	-1.78106	-1.14545
C	10.38323	-0.94641	-2.16765
C	8.88203	-1.22426	-2.11564
N	8.13575	-0.38037	-3.0501
O	6.73701	-0.01922	-4.89277
C	7.43358	-0.92376	-4.08394
O	7.34632	-2.13288	-4.3413
H	12.76392	-2.50594	-0.40421
H	12.78434	-2.24222	-2.16518
H	12.89177	-0.84921	-1.04937
H	10.6085	0.09295	-1.96264
H	10.78248	-1.20468	-3.15087
H	8.69303	-2.26268	-2.37094
H	8.52661	-1.05843	-1.10216
H	7.90788	0.57315	-2.78838
C	7.11886	1.3969	-5.02551
H	6.88204	1.63757	-6.0595
H	8.19078	1.51249	-4.86318
C	6.32529	2.28007	-4.07583
H	5.27568	1.98245	-4.11916
O	6.84341	2.04556	-2.73113
H	6.13204	2.04268	-2.04862
N	9.91823	1.60547	1.47966
C	6.00127	-2.04746	4.5514
O	6.87262	-1.26812	3.69501
C	10.37245	1.12297	2.65661
O	11.47917	1.32269	3.16601
O	9.38634	0.31606	3.31098
C	9.05144	-0.99036	2.65863
C	10.32209	-1.75418	2.26382
O	9.9927	-2.77833	1.27958
C	8.23095	-1.78371	3.65025
H	5.00621	-1.64778	4.40576
H	6.02014	-3.10427	4.2717
H	6.28086	-1.94148	5.60492
H	8.46266	-0.77606	1.7676
H	11.06593	-1.07063	1.85557
H	10.75982	-2.24236	3.1342
H	10.27635	-2.49251	0.37646
H	8.19487	-2.82811	3.33055

H	8.70117	-1.70986	4.63707
C	10.73862	2.47288	0.63574
H	11.24834	1.89648	-0.14524
H	11.50686	2.9355	1.25003
C	9.87768	3.54266	-0.0269
H	9.05878	3.10221	-0.59372
H	9.44174	4.20675	0.72448
O	10.7562	4.27244	-0.92197
C	10.07691	5.30295	-1.6772
H	9.61041	6.04446	-1.01984
H	10.8348	5.78793	-2.28611
H	9.30923	4.86635	-2.32521
H	8.94571	1.43802	1.21319
C	4.84856	1.17427	0.50966
C	6.09536	1.77446	1.14985
C	6.07199	1.61807	2.66894
O	7.22707	2.21281	3.30509
O	7.2618	1.05423	0.61777
H	4.69628	0.16391	0.89682
H	6.19323	2.82913	0.8851
H	5.19452	2.145	3.04559
H	6.00535	0.55358	2.92019
H	7.90716	1.52908	3.46508
H	7.05128	0.80886	-0.29951
H	3.96469	1.77432	0.703
O	5.09946	1.07006	-0.93478
C	4.27968	0.07228	-1.6243
H	3.22774	0.35593	-1.59172
H	4.6247	0.04711	-2.65344
H	4.42279	-0.91065	-1.17308
N	1.274	1.90359	3.54058
C	0.88395	0.56419	4.01078
C	1.97145	-0.4691	3.68957
N	1.57078	-1.84371	4.04406
C	1.92745	-2.86332	3.03401
C	0.94256	-2.85123	1.86943
N	1.31432	-3.75709	0.75458
C	0.1538	-4.0161	-0.11113
C	0.34778	-5.17344	-1.09273
N	-0.89161	-5.36227	-1.86984
C	-0.78378	-6.29364	-3.0058
C	1.80177	-2.23635	5.44257
C	0.65465	-3.07754	6.01606
N	0.95532	-3.47856	7.39644
C	2.52591	-3.30299	0.01876
C	3.65318	-4.34863	0.00138
N	4.91142	-3.81361	-0.55685
C	6.01907	-3.68539	0.41821
C	5.30079	-4.29832	-1.89077
C	4.40337	-3.77489	-3.02335
N	4.97069	-4.16567	-4.31555
C	6.69838	-5.01037	0.83008
N	7.73986	-4.75311	1.83787
H	0.45845	2.48478	3.37407
H	1.93499	2.36726	4.15107

H	-0.0158	0.28213	3.4982
H	0.64989	0.52628	5.08512
H	2.90604	-0.17889	4.19207
H	2.16755	-0.42594	2.6192
H	2.94705	-2.72575	2.66809
H	1.8935	-3.84747	3.50143
H	-0.01482	-3.17599	2.26698
H	0.80346	-1.82797	1.50373
H	-0.69288	-4.25725	0.53603
H	-0.12742	-3.11448	-0.67447
H	1.14586	-4.94843	-1.80209
H	0.64821	-6.07618	-0.54051
H	-1.65951	-5.60651	-1.26139
H	-1.75393	-6.38987	-3.49158
H	-0.0828	-5.89244	-3.73787
H	-0.43635	-7.29811	-2.7208
H	1.88992	-1.33824	6.05293
H	2.74558	-2.78789	5.55508
H	0.45279	-3.92572	5.34448
H	-0.24413	-2.46009	6.02078
H	0.14888	-3.70633	7.95882
H	1.67976	-4.17822	7.48378
H	2.91589	-2.40081	0.48423
H	2.26524	-3.02081	-1.01003
H	3.32204	-5.22928	-0.56101
H	3.81364	-4.68654	1.02811
H	5.64125	-3.19947	1.31819
H	6.77503	-3.01612	-0.00258
H	5.32094	-5.39509	-1.95754
H	6.3162	-3.94845	-2.08472
H	4.28808	-2.68727	-2.89569
H	3.40439	-4.2129	-2.93307
H	4.31628	-4.13214	-5.08411
H	5.82634	-3.6659	-4.53519
H	7.07569	-5.51427	-0.07224
H	5.9511	-5.67215	1.275
H	8.08626	-5.59461	2.28271
H	8.51051	-4.17263	1.5124
C	5.48063	5.88337	-3.68872
H	5.22701	6.20279	-4.70527
H	4.73192	6.25576	-2.99634
H	6.46086	6.28768	-3.41784
C	6.40553	3.75874	-4.42836
H	6.13712	3.91715	-5.48097
H	7.4218	4.13497	-4.26185
O	5.45838	4.43742	-3.57022
C	0.76617	1.69591	-0.19727
O	-0.44515	1.37762	-0.9358
C	-1.15723	2.53059	-1.45047
C	-2.4501	1.99916	-2.06475
N	-3.31064	3.08893	-2.52934
O	-4.5607	4.25834	-4.12267
C	-3.77838	3.12999	-3.80789
O	-3.59222	2.28133	-4.68691
H	1.17468	0.75351	0.1041

H	1.48221	2.2258	-0.83395
H	0.55747	2.28483	0.69593
H	-1.36963	3.23633	-0.63901
H	-0.5555	3.04512	-2.20691
H	-2.22628	1.36056	-2.91424
H	-2.96142	1.39316	-1.3187
H	-3.79974	3.65024	-1.8379
C	-4.38	5.54122	-3.43617
H	-4.49742	6.29063	-4.21666
H	-3.3735	5.6064	-3.0205
C	-5.41699	5.763	-2.34911
H	-6.41782	5.60866	-2.75716
O	-5.17474	4.77864	-1.295
H	-5.68343	5.02514	-0.48875
N	-3.46914	3.37463	1.87785
C	-6.50945	-0.92106	3.9177
O	-5.71239	-0.03005	3.09513
C	-2.60035	2.58487	2.56193
O	-1.49389	2.98767	2.97081
O	-3.02009	1.30054	2.88484
C	-3.62463	0.36937	1.89763
C	-2.48055	-0.33891	1.153
O	-3.13986	-1.1849	0.17142
C	-4.45224	-0.62712	2.67692
H	-7.4189	-0.38201	4.16805
H	-6.7667	-1.83569	3.37477
H	-5.98012	-1.18507	4.83843
H	-4.25545	0.911	1.19228
H	-1.82573	0.38308	0.67141
H	-1.90947	-0.92148	1.87683
H	-2.5958	-1.60868	-0.5489
H	-4.64434	-1.48743	2.03186
H	-3.88261	-0.94508	3.55655
C	-3.08567	4.74481	1.50364
H	-3.66699	5.02448	0.63043
H	-2.03008	4.76219	1.23961
C	-3.32466	5.75286	2.62393
H	-4.36536	5.72413	2.95854
H	-2.66499	5.53567	3.46871
O	-3.01909	7.06886	2.07242
C	-2.86772	8.10142	3.08127
H	-2.05542	7.85646	3.77153
H	-2.62556	9.01806	2.55078
H	-3.79145	8.2408	3.6519
H	-4.38885	3.05517	1.57862
C	-8.38183	2.27315	1.13965
C	-7.38524	3.26002	1.71768
C	-7.05539	2.98156	3.17339
O	-6.17825	3.99946	3.74199
O	-6.14377	3.16354	0.92414
H	-8.03033	1.25028	1.29907
H	-7.77002	4.27743	1.61296
H	-7.97602	3.0217	3.75579
H	-6.60379	1.99329	3.26615
H	-5.2498	3.74277	3.60248

H	-6.4071	3.0383	-0.01053
H	-9.37223	2.38447	1.58863
O	-8.43455	2.55509	-0.29328
C	-9.42502	1.7705	-1.01788
H	-10.43178	2.04295	-0.68753
H	-9.28711	1.98896	-2.07107
H	-9.25671	0.70321	-0.8569
N	-11.87164	0.878	2.07851
C	-12.03369	-0.38517	1.33388
C	-10.74963	-1.21746	1.42743
N	-10.8149	-2.46905	0.65915
C	-9.52018	-2.93985	0.13179
C	-9.64992	-3.82462	-1.11978
N	-8.34035	-4.19594	-1.67743
C	-8.07457	-5.62174	-1.91007
C	-6.60382	-5.99837	-1.67498
N	-6.39089	-7.43198	-1.89661
C	-4.99884	-7.86512	-2.01531
C	-11.6628	-3.51808	1.2624
C	-12.90727	-3.85902	0.42898
N	-13.70259	-4.8925	1.10657
C	-7.75007	-3.27216	-2.66276
C	-6.6016	-2.41621	-2.09191
N	-5.82754	-1.72371	-3.14061
C	-6.4822	-0.51745	-3.70942
C	-4.40922	-1.4871	-2.78363
C	-3.52544	-2.73013	-2.87334
N	-2.20738	-2.44946	-2.23722
C	-6.4763	0.71721	-2.78939
N	-7.13081	1.86276	-3.44043
H	-12.56156	1.58089	1.84987
H	-11.80687	0.75301	3.08165
H	-12.20706	-0.14925	0.28397
H	-12.8914	-0.9793	1.67802
H	-10.51879	-1.40429	2.49321
H	-9.93918	-0.61817	1.03173
H	-8.9312	-2.06648	-0.13939
H	-8.94221	-3.49764	0.8874
H	-10.19207	-4.73872	-0.86807
H	-10.26132	-3.28348	-1.85576
H	-8.69739	-6.19627	-1.22036
H	-8.33979	-5.93964	-2.92987
H	-5.97506	-5.459	-2.38826
H	-6.3075	-5.66097	-0.66855
H	-6.91756	-8.00219	-1.24336
H	-4.96225	-8.94487	-2.15646
H	-4.5461	-7.40449	-2.89672
H	-4.37822	-7.6164	-1.14372
H	-12.00211	-3.21063	2.25577
H	-11.0694	-4.43081	1.41254
H	-12.59491	-4.12995	-0.58885
H	-13.51916	-2.96091	0.3391
H	-14.67027	-4.9363	0.82154
H	-13.27899	-5.81093	1.10947
H	-8.53875	-2.63207	-3.07286

H	-7.34099	-3.83981	-3.50297
H	-5.92871	-3.08574	-1.55944
H	-6.99446	-1.72041	-1.33436
H	-7.51322	-0.75188	-3.97611
H	-5.96263	-0.26828	-4.63868
H	-4.29625	-1.10527	-1.75618
H	-4.02571	-0.73225	-3.47312
H	-3.42736	-3.0566	-3.91654
H	-3.98543	-3.55076	-2.31973
H	-1.65964	-3.31059	-2.18101
H	-1.68335	-1.76045	-2.7737
H	-5.44456	0.94002	-2.49286
H	-7.02494	0.49032	-1.87404
H	-7.19909	2.66163	-2.82157
H	-6.67131	2.13234	-4.30533
C	-6.04651	8.18813	0.37498
H	-6.19748	9.16679	-0.08857
H	-6.79656	8.03311	1.14423
H	-5.04679	8.1237	0.80944
C	-5.32873	7.15076	-1.72437
H	-5.62153	7.92608	-2.43951
H	-4.30975	7.3462	-1.37365
O	-6.24497	7.12031	-0.59783

Coordinates of large aggregate
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	3.95149	9.7305	-3.85947
O	3.64927	9.08829	-2.5932
C	4.82473	8.71002	-1.79742
C	4.35274	8.54129	-0.35678
N	5.43411	8.07537	0.5119
O	7.4438	8.35287	1.68649
C	6.43754	8.91562	0.87951
O	6.52543	10.10994	0.56563
H	2.9962	9.96379	-4.3225
H	4.51146	10.65336	-3.69271
H	4.52706	9.06772	-4.51173
H	5.22921	7.7712	-2.17467
H	5.56741	9.5069	-1.86112
H	3.95998	9.49343	0.00298
H	3.56678	7.79156	-0.33515
H	5.31737	7.19487	1.00738
C	7.78715	6.92829	1.61733
H	8.8634	6.90562	1.78206
H	7.5629	6.5325	0.62574
C	7.09103	6.10192	2.68168
H	7.1367	6.62804	3.63795

O	5.68689	5.94783	2.2926
H	5.31397	5.22628	2.83586
N	3.52305	3.48003	-0.99972
C	-1.73535	3.41347	-2.80803
O	-0.35667	3.17413	-3.25265
C	3.26418	4.56704	-1.75877
O	3.858	5.66128	-1.7286
O	2.24453	4.25108	-2.66282
C	1.11346	5.15136	-2.96631
C	1.51866	6.51669	-3.52949
O	1.46721	7.51891	-2.4825
C	0.28118	4.31014	-3.92705
H	-2.11227	2.44573	-2.48854
H	-1.74899	4.09913	-1.96347
H	-2.33752	3.78533	-3.64088
H	0.55512	5.30264	-2.04343
H	2.51688	6.45142	-3.96205
H	0.81418	6.80559	-4.31753
H	2.27499	8.0959	-2.48879
H	-0.49209	4.92173	-4.39896
H	0.92256	3.87531	-4.69117
C	4.67089	3.37881	-0.10353
H	4.39663	2.73645	0.73341
H	4.92264	4.36101	0.29172
C	5.88637	2.77157	-0.80412
H	5.60505	1.83886	-1.30739
H	6.28242	3.46483	-1.55446
O	6.88185	2.50283	0.21742
C	8.12858	1.94796	-0.29522
H	8.65343	2.6738	-0.92221
H	8.73286	1.70148	0.57079
H	7.94491	1.03885	-0.87541
H	2.80053	2.75861	-1.00799
C	-0.20293	3.80253	2.28939
C	0.27995	3.71861	0.84713
C	0.29824	2.27894	0.33738
O	1.00286	2.14053	-0.92587
O	-0.57609	4.48142	-0.03482
H	-1.26575	3.54079	2.34662
H	1.30234	4.11183	0.81763
H	0.82232	1.62316	1.0311
H	-0.73108	1.92479	0.22928
H	0.54092	2.58947	-1.67263
H	-0.40964	5.49527	0.03387
H	0.36833	3.11703	2.92956
O	-0.00151	5.16873	2.74769
C	-0.43494	5.39086	4.11335
H	0.11453	4.75017	4.81126
H	-0.22255	6.4321	4.33887
H	-1.50813	5.20534	4.22429
N	-3.15555	0.03809	0.89657
C	-4.38989	0.84105	0.94718
C	-4.42201	2.01257	-0.05417
N	-5.72172	2.70759	-0.0774
C	-5.6753	4.15568	-0.33032

C	-6.84381	4.90652	0.32748
N	-6.74345	6.36708	0.14081
C	-8.03349	7.0758	0.08349
C	-7.96862	8.39526	-0.69503
N	-9.30105	9.00342	-0.77593
C	-9.34867	10.35868	-1.33135
C	-6.78121	1.97058	-0.79708
C	-7.96071	1.52545	0.08264
N	-8.90687	0.71671	-0.71026
C	-5.71959	7.02298	0.9839
C	-4.62128	7.75332	0.18089
N	-3.582	8.32859	1.04907
C	-2.29307	7.62622	1.09057
C	-3.55303	9.78976	1.18428
C	-4.6942	10.33906	2.05561
N	-4.58414	11.79707	2.17487
C	-1.35639	7.91679	-0.09876
N	-0.11075	7.11798	-0.0074
H	-3.11835	-0.55366	0.06738
H	-2.3162	0.60057	0.98616
H	-4.53365	1.24299	1.95211
H	-5.22447	0.16894	0.74988
H	-4.15251	1.61899	-1.04943
H	-3.64976	2.73334	0.2252
H	-4.73824	4.53612	0.07794
H	-5.68032	4.3945	-1.40789
H	-7.77923	4.57497	-0.12477
H	-6.88006	4.62236	1.39057
H	-8.74879	6.41952	-0.41926
H	-8.4387	7.28952	1.08585
H	-7.31802	9.1035	-0.17604
H	-7.51137	8.20216	-1.67937
H	-9.97231	8.38594	-1.22033
H	-10.3812	10.70858	-1.35001
H	-8.7834	11.0363	-0.68856
H	-8.93624	10.44516	-2.35046
H	-6.35599	1.06755	-1.24231
H	-7.15811	2.58436	-1.6297
H	-8.43152	2.40261	0.54449
H	-7.58649	0.91116	0.89976
H	-9.41582	0.02486	-0.17634
H	-9.53616	1.25329	-1.29396
H	-5.23239	6.27433	1.61495
H	-6.19435	7.7344	1.67067
H	-5.07315	8.54076	-0.42982
H	-4.18242	7.03932	-0.52286
H	-2.47792	6.55221	1.13892
H	-1.78105	7.89142	2.02126
H	-3.58974	10.3097	0.21586
H	-2.60357	10.06351	1.65347
H	-4.68171	9.80186	3.01503
H	-5.65139	10.11637	1.57901
H	-5.43725	12.27058	2.43451
H	-3.79883	12.11448	2.72739
H	-1.14635	8.99185	-0.14603

H	-1.85514	7.64864	-1.03244
H	0.51393	7.30357	-0.79903
H	0.37464	7.26651	0.87337
C	6.9925	2.55396	3.75864
H	8.0159	2.30665	4.04306
H	6.2962	2.17189	4.50048
H	6.78599	2.12545	2.77696
C	7.6864	4.70605	2.82749
H	8.69442	4.74752	3.25283
H	7.71075	4.19496	1.86154
O	6.78373	4.00206	3.72756
C	-7.266	1.07582	4.04247
O	-7.40881	-0.09318	3.18828
C	-6.43274	-1.13777	3.45789
C	-6.7117	-2.27904	2.48368
N	-5.83598	-3.4284	2.72876
O	-5.2085	-5.37331	3.8706
C	-6.11092	-4.31111	3.71993
O	-7.08154	-4.25274	4.49253
H	-8.11945	1.71687	3.83977
H	-7.27598	0.78503	5.09823
H	-6.33598	1.60774	3.82194
H	-5.41691	-0.75592	3.31478
H	-6.54203	-1.49069	4.48817
H	-7.7518	-2.58348	2.58113
H	-6.54585	-1.94543	1.46083
H	-5.17052	-3.6992	2.00778
C	-3.80151	-5.25866	3.4638
H	-3.2603	-5.8349	4.21291
H	-3.46959	-4.22019	3.49279
C	-3.55011	-5.83964	2.08513
H	-4.02023	-6.82239	2.00308
O	-4.15829	-4.94244	1.10281
H	-3.7134	-5.0739	0.24393
N	-4.25452	-3.70789	-2.41162
C	-3.53071	0.30832	-4.92973
O	-4.31453	-0.84361	-4.53247
C	-4.32442	-2.42977	-1.97925
O	-3.39955	-1.8097	-1.4211
O	-5.58493	-1.82807	-2.11688
C	-6.24127	-1.74277	-3.44562
C	-7.74256	-1.66756	-3.20133
O	-8.29497	-2.9727	-2.88069
C	-5.68699	-0.53427	-4.17799
H	-2.51155	-0.0415	-5.06585
H	-3.90183	0.73742	-5.86686
H	-3.54296	1.07578	-4.15048
H	-5.9995	-2.63538	-4.02428
H	-7.9672	-0.94587	-2.41176
H	-8.23453	-1.34815	-4.12126
H	-8.38422	-3.16185	-1.91163
H	-6.27222	-0.33831	-5.08516
H	-5.72719	0.34533	-3.52908
C	-2.99581	-4.45178	-2.37051
H	-3.23087	-5.51483	-2.3505

H	-2.4502	-4.20256	-1.46217
C	-2.09783	-4.16093	-3.56884
H	-2.61685	-4.38969	-4.50602
H	-1.80297	-3.10768	-3.57567
O	-0.92808	-5.01596	-3.41858
C	0.08837	-4.8005	-4.42998
H	0.48477	-3.78221	-4.37947
H	0.88593	-5.50838	-4.22036
H	-0.30804	-4.98738	-5.43385
H	-5.11637	-4.21759	-2.64014
C	-8.03495	-6.39102	0.49845
C	-7.46055	-5.38232	-0.49633
C	-7.27016	-6.00344	-1.87445
O	-6.67272	-5.0861	-2.83622
O	-8.4227	-4.26951	-0.59903
H	-8.83915	-6.97172	0.03269
H	-6.51946	-4.9819	-0.11706
H	-6.58372	-6.8473	-1.79308
H	-8.23122	-6.36422	-2.24978
H	-7.32943	-4.37879	-3.07902
H	-8.83118	-4.16839	0.28539
H	-7.25421	-7.07056	0.85351
O	-8.57341	-5.61173	1.59968
C	-9.23215	-6.40069	2.63651
H	-8.50252	-7.03579	3.14433
H	-9.66007	-5.69715	3.34506
H	-10.02028	-7.01968	2.19537
N	-10.44731	-7.3366	-2.88369
C	-11.66514	-6.64441	-2.42183
C	-11.5287	-5.13575	-2.65625
N	-12.69335	-4.38012	-2.16554
C	-12.42048	-2.99322	-1.74695
C	-13.26627	-2.57879	-0.5335
N	-13.05435	-1.16756	-0.15155
C	-13.8307	-0.20147	-0.95266
C	-13.06707	1.10378	-1.20144
N	-13.89466	2.06056	-1.94175
C	-13.32576	3.39906	-2.108
C	-13.93509	-4.56879	-2.9397
C	-15.01654	-5.37594	-2.20297
N	-16.20487	-5.52416	-3.05391
C	-13.1045	-0.92473	1.30701
C	-11.75321	-1.19688	1.98903
N	-11.81151	-1.00619	3.45096
C	-11.62325	-2.23151	4.25458
C	-11.09167	0.17684	3.95698
C	-11.74801	1.50455	3.5601
N	-10.97111	2.62649	4.1112
C	-10.16412	-2.70869	4.3548
N	-10.05542	-4.01007	5.0326
H	-10.4239	-8.3225	-2.65603
H	-10.24734	-7.18992	-3.86646
H	-11.77732	-6.81469	-1.35031
H	-12.57602	-7.01886	-2.90961
H	-11.35355	-4.95463	-3.73322

H	-10.64135	-4.79359	-2.12836
H	-11.3697	-2.90765	-1.47436
H	-12.5882	-2.28507	-2.5756
H	-14.33234	-2.77719	-0.72874
H	-12.98206	-3.21753	0.30261
H	-14.05485	-0.66298	-1.91774
H	-14.79587	0.04131	-0.48393
H	-12.80353	1.56139	-0.24396
H	-12.11737	0.86162	-1.70859
H	-14.23192	1.67593	-2.81766
H	-14.01578	4.02151	-2.67818
H	-13.1957	3.86456	-1.12885
H	-12.3467	3.41481	-2.61762
H	-13.72398	-5.07689	-3.88668
H	-14.3502	-3.58725	-3.20558
H	-15.21704	-4.89886	-1.23356
H	-14.62586	-6.37101	-1.98753
H	-16.8162	-6.28652	-2.79824
H	-16.72413	-4.66791	-3.19816
H	-13.87998	-1.53526	1.79308
H	-13.37988	0.11579	1.47969
H	-11.	-0.53666	1.54422
H	-11.43683	-2.21867	1.75722
H	-12.22851	-3.02991	3.82163
H	-12.01999	-2.04493	5.25885
H	-10.04658	0.20023	3.62454
H	-11.08324	0.11196	5.04936
H	-12.80002	1.48768	3.87755
H	-11.74027	1.60485	2.47273
H	-11.13988	3.51746	3.66558
H	-11.01576	2.70441	5.11925
H	-9.56162	-1.92524	4.834
H	-9.76545	-2.83175	3.34656
H	-9.08601	-4.31391	5.07653
H	-10.47729	-4.01471	5.95541
C	-0.61652	-6.36472	-0.15708
H	-0.14789	-7.28327	0.20813
H	-0.70314	-6.3842	-1.23888
H	-0.01254	-5.50247	0.13609
C	-2.0585	-5.95113	1.7855
H	-1.60247	-6.75286	2.37648
H	-1.55795	-5.00232	2.00122
O	-1.97174	-6.2469	0.36426
C	14.60687	-3.39593	3.38809
O	14.06431	-3.79042	2.09427
C	12.75394	-4.41348	2.17542
C	12.29182	-4.68143	0.74493
N	11.03963	-5.44839	0.71798
O	8.70977	-5.6373	0.89753
C	9.85077	-4.83583	0.88718
O	9.69977	-3.6067	1.04626
H	15.57218	-2.94167	3.18814
H	13.95417	-2.66763	3.87399
H	14.73663	-4.27084	4.03079
H	12.82695	-5.35392	2.73278

H	12.05142	-3.74803	2.68401
H	12.15803	-3.73532	0.22352
H	13.05154	-5.2598	0.22268
H	11.05918	-6.41117	0.3816
C	8.73781	-7.06014	1.26121
H	7.74438	-7.23524	1.66843
H	9.48675	-7.23691	2.03471
C	8.9888	-7.97582	0.07627
H	8.47551	-7.58322	-0.80431
O	10.42956	-7.99603	-0.16886
H	10.62407	-8.69487	-0.82048
N	14.71287	-1.40618	0.55407
C	12.42	3.11214	-0.78726
O	11.72192	1.92073	-0.32431
C	14.00971	-0.26288	0.73327
O	14.32177	0.84757	0.26926
O	12.91899	-0.49297	1.57784
C	11.6311	0.24755	1.44234
C	10.92735	0.00624	2.78323
O	9.58162	0.52753	2.75533
C	11.75937	1.72859	1.13015
H	12.34992	3.10039	-1.87154
H	11.94232	4.01525	-0.39722
H	13.46512	3.06566	-0.48416
H	11.07082	-0.24227	0.64444
H	10.93908	-1.06777	2.98709
H	11.46754	0.51498	3.58291
H	8.93647	-0.15356	2.36487
H	10.89975	2.24438	1.56164
H	12.68525	2.13604	1.53216
C	15.89886	-1.43241	-0.30024
H	16.52641	-2.27125	-0.00105
H	16.46385	-0.51228	-0.16237
C	15.53312	-1.56632	-1.77746
H	14.97204	-2.49357	-1.95139
H	14.91222	-0.72453	-2.09366
O	16.78904	-1.59773	-2.51062
C	16.62457	-1.58271	-3.94727
H	16.08827	-0.68652	-4.27632
H	17.62502	-1.58339	-4.37238
H	16.08166	-2.46888	-4.29713
H	14.37214	-2.26285	0.97996
C	9.5871	-2.61886	-3.01165
C	10.56123	-1.85863	-2.12605
C	11.04405	-0.5629	-2.76675
O	12.23534	-0.05252	-2.13575
O	9.92728	-1.51861	-0.85899
H	8.68266	-2.02551	-3.18348
H	11.43505	-2.49244	-1.94356
H	11.30069	-0.7555	-3.81105
H	10.23025	0.16855	-2.73644
H	12.02826	0.59854	-1.41937
H	9.80318	-2.32282	-0.30935
H	10.05102	-2.84844	-3.98021
O	9.24022	-3.85299	-2.32604

C	8.2235	-4.6313	-3.01335
H	8.63336	-5.09652	-3.91759
H	7.91185	-5.4051	-2.31629
H	7.36712	-4.01	-3.28998
N	5.78015	-2.37186	-4.94466
C	4.38447	-2.08222	-4.5654
C	4.3532	-1.39859	-3.19433
N	2.99334	-1.10737	-2.72046
C	2.81423	-1.12455	-1.25441
C	1.51094	-1.82099	-0.8334
N	1.35528	-1.89615	0.63519
C	-0.02746	-2.16066	1.07755
C	-0.30027	-1.68564	2.50894
N	-1.6924	-1.95126	2.90098
C	-1.98867	-1.58809	4.29252
C	2.31176	0.00462	-3.42096
C	1.14003	-0.43599	-4.31257
N	0.54292	0.73611	-4.96258
C	2.37837	-2.72045	1.31551
C	3.34043	-1.89518	2.19619
N	4.43671	-2.70839	2.74718
C	5.73072	-2.61589	2.0566
C	4.46755	-2.90117	4.20128
C	3.37271	-3.85825	4.70054
N	3.46712	-4.03047	6.15323
C	6.58569	-1.3747	2.40931
N	7.88054	-1.31808	1.69417
H	5.87089	-3.00226	-5.73084
H	6.34166	-1.5401	-5.08476
H	3.84299	-3.02583	-4.48851
H	3.85902	-1.46227	-5.30405
H	4.97211	-0.48163	-3.24346
H	4.8377	-2.07165	-2.48785
H	3.66024	-1.65957	-0.82184
H	2.81472	-0.11084	-0.83373
H	0.66643	-1.25734	-1.22955
H	1.4891	-2.8193	-1.30256
H	-0.70481	-1.64422	0.39653
H	-0.27723	-3.23254	1.01404
H	0.35543	-2.21335	3.20893
H	-0.03475	-0.61611	2.57844
H	-2.34262	-1.48248	2.2619
H	-3.04846	-1.74711	4.49218
H	-1.41883	-2.22108	4.97761
H	-1.75119	-0.53871	4.53708
H	3.02513	0.55157	-4.04664
H	1.93547	0.71441	-2.67997
H	0.43344	-1.01468	-3.69844
H	1.51225	-1.11112	-5.08662
H	-0.05255	0.53709	-5.75265
H	0.15343	1.43362	-4.3366
H	2.97167	-3.27278	0.57813
H	1.89555	-3.48005	1.93932
H	2.7747	-1.43336	3.0103
H	3.73277	-1.06774	1.59619

H	5.54745	-2.62767	0.97867
H	6.31421	-3.51614	2.27372
H	4.37213	-1.96101	4.76354
H	5.44105	-3.32732	4.46175
H	3.44825	-4.79342	4.12624
H	2.39337	-3.42818	4.47919
H	2.61448	-4.31018	6.61444
H	4.26237	-4.56892	6.46766
H	6.79048	-1.36834	3.48202
H	6.0345	-0.45947	2.18699
H	7.78608	-1.04733	0.71951
H	8.38766	-2.20195	1.72286
C	8.75317	-11.58787	-0.76701
H	7.67662	-11.77802	-0.76265
H	9.19231	-12.00855	-1.6661
H	9.20935	-12.04581	0.11533
C	8.53123	-9.40801	0.32581
H	7.43939	-9.46668	0.38489
H	8.9663	-9.79855	1.25283
O	9.02569	-10.16075	-0.81309