Electronic Supplementary Material (ESI) for RSC Advances.

Green alternative cosolvents to NMP in water polyurethane dispersions (PUD).

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Supplementary information

Solvents Health, Environmental and Safety (HES) information

Health, environmental impact and safety data of N-Methyl-2-pyrrolidone (NMP) and alternative green solvents: Dihydrolevoglucosenone (CY) and ɣ-Valerolactone (GVL) are summarized in Table S1. Scores are assigned on a scale from 1 to 10, with the intent that the solvent rated the least green in a category has score equal to 1, and that rated the greenest has score equal to 10.

All this information is based on following solvent selection guides:

- CHEM21 Innovative Medicines Initiative (IMI)-CHEM21 public- private partnership is a European consortium which promotes sustainable biological and chemical methodologies.
- GSK's solvent sustainability guide.

Table S1. Data about health, environmental impact and safety of solvents[1 2 3 4]

SOLVENT	Boiling point(ºC)	Health Hazard	Exposure potential	Aquatic impact	Air impact	Reactivity and stability
NMP	202	1	9	10	6	10
CY	203	4	8	9	6	10
GVL	207	4	8	10	6	10

Characterization of PUDs

Conversion of NCO groups by Fourier-Transform Infrared spectroscopy (FTIR)

Quantification of the conversion of NCO groups is based on Beer-Lambert law and calculated from decay in the corresponding absorbance. The area below the isocyanate stretch peak located at ~2260 cm^{-1}, thus, is measured, and the result is normalized with respect to the area below the C–H stretch peaks between ~2840 and ~3050 cm^{-1}. The conversion of the isocyanate functional group as a function of time was calculated from

$$Conversion = 1 - \frac{A_t}{A_0}$$

where A_t is the normalized area under the isocyanate peak at different reaction times t and A_0 is the initial normalized area under the isocyanate peak (t=0)[5 6].

Table S2. Experimental data of NCO conversion analysis.

NCO Conversion*			
TIME	**PUD_NMP**	**PUD_CY**	**PUD_GVL**
0	0.00	0.00	0.00
150	0.67±0.04	0.57±0.01	0.65±0.01
180	0.76±0.03	0.650.03±	0.71±0.01
270	0.91±0.03	0.86±0.05	0.92±0.02

* Values are mean of three replicates

Polyurethane films

Film fabrication

Fabrication of polyurethane transparent films, Figure S1.

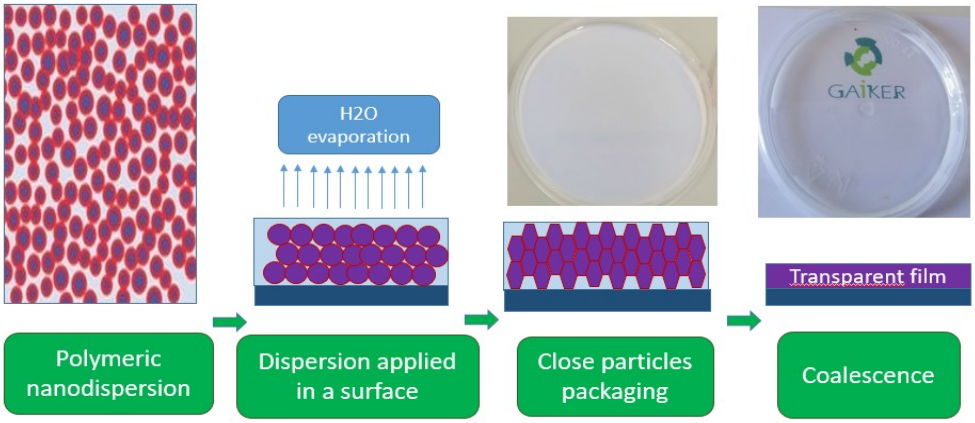
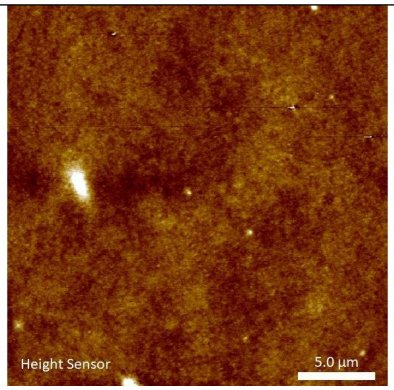
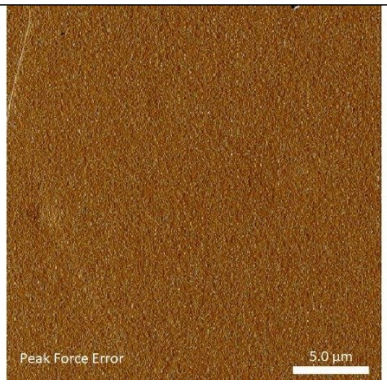
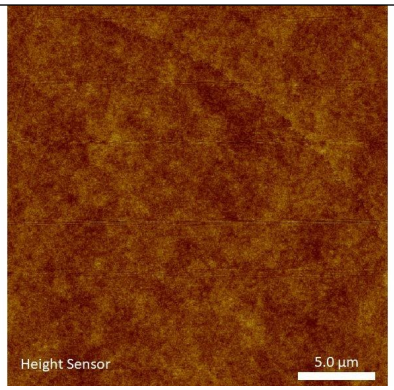
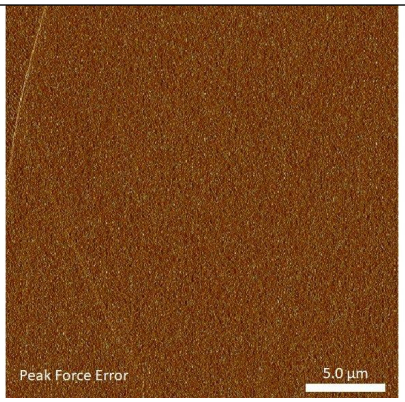
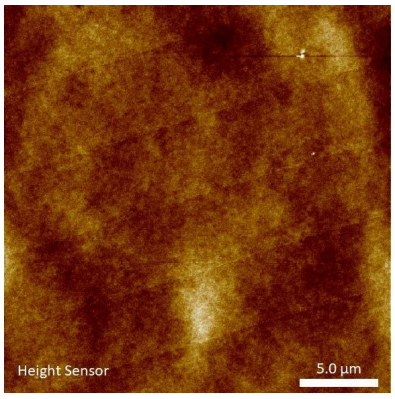
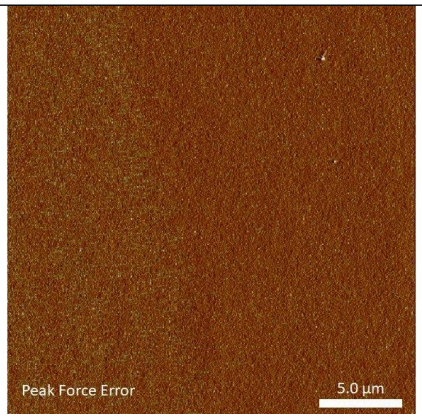


Figure S1. PUD forming transparent films.

Atomic Force Microscopy (AFM) surface quality

Surface topography of polyurethane films (Table S3).

Table S3. AFM images of polyurethane films surfaces

HEIGHT IMAGE	PHASE IMAGE
	
PUD_NMP	
	
PUD_CY	
	
PUD_GVL	

Dynamic mechanical analysis (DMA)

Dynamic mechanical thermal properties measured by DMA..

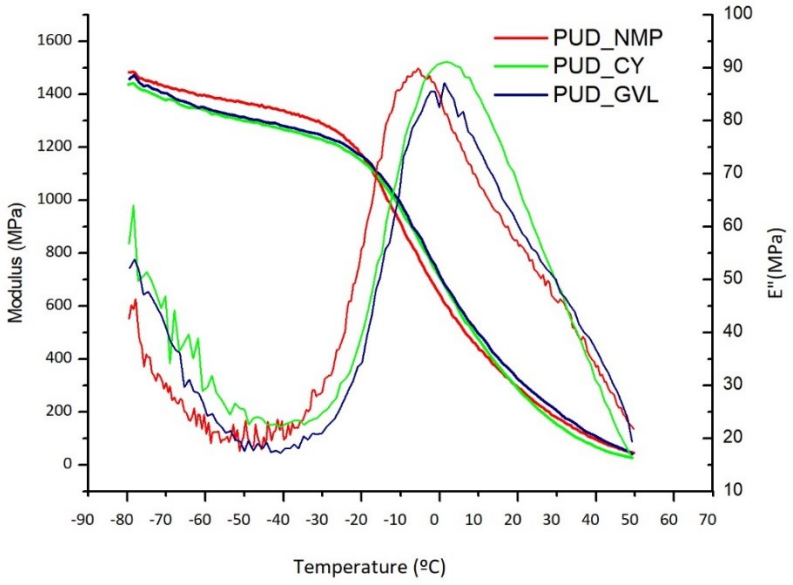


Figure S2. DMA of PU materials synthesized with different cosolvent.

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