Electronic Supplementary Material (ESI) for ChemComm.

Hue-based quantification of mechanochromism towards a cost-effective detection of mechanical strain in polymer systems

- ELECTRONIC SUPPLEMENTARY INFORMATION -

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1. Conversion from RGB to HSV colour space

RGB images can be easily converted to HSV stacks by mathematical elaboration based on the three R, G and B values of the original image. The mathematical piecewise equations used to obtain the HSV values from a RGB image are the following:

$$R' = \frac{R * 100}{255}$$

$$G' = \frac{G * 100}{255}$$

$$B' = \frac{B * 100}{255}$$

$$M = \frac{\max(R, G, B) * 100}{255}$$

$$m = \frac{\min(R, G, B) * 100}{255}$$

$$H' = \frac{\frac{G' - B'}{M - m} + 0}{6} \qquad if\ R = max$$

$$H' = \frac{\frac{B' - R'}{M - m} + 2}{6} \qquad if\ G = max$$

$$H' = \frac{\frac{R' - G'}{M - m} + 4}{6} \qquad if\ B = max$$

$$H = H' * 360°$$

$$S = \frac{M - m}{M}$$

$$V = M$$

It is worth noting that neutral colours (greys) are undefined in this space, since R = G = B and (M – m) = 0; actually, the grey scale is given by any colour showing a 0% value for S and a V ranging from 0% (black) to 100% (white).

2. Spectral centre of gravity (CG) calculation

The centre of gravity (λ_{CG} or CG) of the fluorescence spectra was calculated according to the following equation:

$$\lambda_{CG} = \frac{\int \lambda I(\lambda) d\lambda}{\int I(\lambda) d\lambda}$$

where λ is the wavelength and $I(\lambda)$ the fluorescence intensity. Accordingly, the spectral centre of gravity obtained for the different BBS/LLDPE films is shown in Table 1, along with the hue values obtained from the conversion to HSV and the relevant wavelengths calculated from the calibration line (see main text).

Stretching ratio	Hue (°)[a]	Wavelength (nm)[b]	CG (nm)[c]
1:1 (not stretched)	170.6	500	507.3
2:1	189.6	484	503.9
3:1	202.6	473	473.6
4:1	220.2	457	465.8
5:1	215.7	461	450.6
6:1	216.0	461	458.9

Table 1: [a] Average hue values calculated from the conversion of RGB images to HSV stacks; [b] Wavelengths calculated from the hue/wavelength calibration line; [c] Wavelengths calculated for the spectral centre of gravity from the fluorescence spectra.

3. Preparation of BBS/LLDPE films

Linear low-density polyethylene (LLDPE, Dowlex SC 2107, melt flow index 190°C/2.16 kg 2.3 g/10 min, d = 0.917 g/cm^3, supplied by Dow Plastics, USA) was used as the polymer host matrix. 4,4'-bis-(2-benzoxazolyl) stilbene (BBS) was supplied by Aldrich and used without further purification.
BBS/LLDPE blends were prepared in a Brabender plastograph mixer (mod. OHG47055, 30 cm^3) under nitrogen atmosphere by introducing about 20 g of the polymer and 0.3% wt of BBS in the mixer at 180 °C setting the rotor speed at 50 rpm. After 10 min, the mixing was stopped and the recovered material was moulded between two aluminium foils under compression in a Collin mod. 200 M press (Dr. Collin GmbH, Ebersberg, GE) at 180 °C for 5 min. After removal from the press, the films were allowed to slowly reach room temperature (about 5 °C·min^{-1}). The films were generally analysed after 2-3 days. The thickness of the obtained films was in the range of 80-100 µm.

4. Preparation, spectroscopic characterization and imaging of the stretched BBS/LLDPE films

Solid-state stretching of the binary films was performed at room temperature or at 60 °C on a thermostatically controlled hot stage. The stretching ratio, defined as the ratio between the final and the initial length of the samples, was determined by measuring the displacement of ink-marks printed on the films before stretching. Samples were stretched according to definite stretching ratios, from 1:1 (not stretched) to 6:1 (*i.e.* six times the original length).
Steady-state fluorescence spectra of BBS/LLDPE films were acquired at room temperature under isotropic excitation at 360 nm with a Horiba Jobin–Yvon Fluorolog®-3 spectrofluorometer equipped with a 450 W xenon arc lamp, double-grating excitation and single-grating emission monochromators and the Front Surface Accessory.
Digital images were taken using the on-board camera of a Nokia Lumia 635 mobile phone (main camera pixel resolution: 5.0 MP, f-number/aperture: f/2.4, camera focal length: 28 mm) by exposing the films under a Camag UV-Cabinet II equipped with Sylvania 8W long-range lamps (λ = 366 nm).

5. Confocal fluorescence microscopy

Confocal fluorescence imaging of BBS/LLDPE films was performed using a Leica TCS SP5 inverted confocal microscope (Leica Microsystems AG, Wetzlar, Germany) equipped with an external pulsed diode laser for excitation at 405 nm and a built-in acousto-optical beam splitter (AOBS) detection system. Laser repetition rate was set to 40 Hz. Image size was 512x512 pixels and scan speed was usually set to 400 Hz (lines per second). The pinhole aperture was set to 1.0 Airy. Samples were fixed to a microscope glass slide and imaged using a HC PL Fluotar 20.0x 0.5 numerical aperture dry objective (Leica Microsystems). The pinhole aperture was set to 1 Airy (84.9 µm confocal aperture). For all samples, emission was monitored in the 415-455 and 490-580 nm ranges using the integrated AOBS detection system.