Experimental report

25/05/2018

Proposal: 9-10-1523 **Council:** 4/2017

Title: Magnetic Alignment of Photoconductive Perylene Bisimides

Research area: Materials

This proposal is a resubmission of 9-10-1494

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Samples: perylene bisimide phenylalanine
perylene bisimide alanine
perylene bisimide histidine

Instrument	Requested days	Allocated days	From	To
D11	0	0		
D33	3	3	13/04/2018	16/04/2018

Abstract:

Aligned materials are very important for developing small organic molecules for the use in electronics. Aligning materials makes devices like OPVs work more efficiently and allows for flexible devices. We are using low molecular weight gelators to form worm-like micelles and gel fibres that are photoresponsive. We have already used shear alignment and have preliminary work of magnetically aligned samples showing they align perpendicular to the field. Magnetic alignment is advantageous as it allows the structures to be aligned in different directions. We find there is a great improvement on performance and directional dependence of the photocurrent produced in aligned samples. We will use SANS to probe both the worm-like micelles and gel fibres under a large magnetic field. The strength of the magnetic field required to create an aligned system will be investigated along with the effect of the increased exposure to the field on the alignment over time. We will then compare to previous SANS data to see if the field has effected the structures. We will investigate whether the structures stay aligned after being removed from the field, and if they de-align, how long this process takes.

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Abstract Perylene bisimides (PBIs) are of great interest due to their electronic properties. When irradiated with the right wavelength of light they become conductive due to the formation of a radical anion. This conductive behaviour means that these materials can be used in devices such as transistors and solar cells. To improve the conductivity the materials can be aligned to ensure reduced recombination of the charges responsible for the conductivity of the materials, by providing a shorter, more direct path for the electrons travel through the material. This can be done by an external force such as shear, or a magnetic field. Here we look at the effect of magnetic field strength on the PBI structures and the alignment of them in solution.

Introduction PBIs are photoconductive molecules which are able to except an electronic into their conjugated core, meaning they are very good n-type materials for electronics. Amino acid functionalized PBIs are able to pi-pi stack in water to form long fibre like structures, called worm-like-micelles. These structures are advantageous as it allows the electrons generated by exposure to light to travel along these fibres like a molecular wire. We have previously shown that when aligned these materials are more conductive and directionally dependent. This was done using a shear force but resulted in a circularly aligned sample.[1] We have previously shown for worm-like micelles made from low molecular weight gelators (LMWGs) that they are also able to align the worm-like micelles perpendicular to a magnetic field.[2] This alignment can be seen in NMR spectra, with the ^{23}Na peak becoming split with increasing alignment due to residual quadrupolar coupling. This method would allow a non-contact method for aligning the PBIs in one direction rather than circularly. We have previously collected proof of principle data using the NMR technique, showing that these PBIs to align in the presence of a magnetic field. We aimed to determine whether the magnetic field has an effect on the structures and what strength field Is needed for them to align. We will then dry these samples under a magnetic field and measure the conductivity and directional dependence of the samples.

Experimental The LMWG were prepared as described elsewhere.[1] Solutions at 10 mg/mL, 30 mg/mL and 50 mg/mL were prepared in D_2O at high pD by the addition of one molar equivalent of NaOD (0.1 M), followed by stirring until the LMWG had dissolved. SANS experiments were performed on the D33 diffractometer, a neutron wavelength of λ= 10 Å was employed at a detector distance of, D = 1.1m and 8 m. All spectra were normalised and corrected using the scattering of the empty cell. Scattering data were corrected for electronic noise and incoherent background subtraction and normalised by the intensity scattered for a 1 mm H_2O sample corrected by the intensity scattered from the empty quartz cell. The scattering of each of the solutions was then measured in the presence of a magnetic field, provided by a cryo-magnet. Each solution was exposed to 0-8 T in increments of 1 T, then held at 8 T before being lowered to 0 T again.

Results The PBI worm-like micelles at each concentration fit to a flexible cylinder model, this did not change once exposed to the different magnetic field strengths, so the structures themselves were not affected by the magnetic field. However, the scattering pattern itself became anisotropic in nature with the pattern become radially stretched along the x-axis. This is due to the worm-like micelles becoming aligned perpendicular to the magnet field. The amount of anisotropy was directly proportional to the field strength in all cases. This meant the at 8 T the samples were the most anisotropic and therefore aligned and 0 T were isotropic, and so not aligned. The amount of alignment was not dependent on whether the field strength was decreasing or increasing and did not change if held at a specific field strength for a long time. When the magnetic field was removed, the samples became isotropic again almost immediately. This very quick relaxation time means that these samples must be dried or gelled under the magnet field in order to maintain the alignment achieved using the magnet. These data are currently being analysed and are in the process being written up for a publication.

References

1. E. R. Draper et al., *Chem. Commun.*, **2016**, *52*, 6934.
2. M. Wallace et al., *Chem, Eur. J.*, **2014**, *20*, 16484-16487