

Fluorescence Polarization Measurements to Probe Alignment of a Bithiophene Dye in One-Dimensional Channels of Self-Assembled Phenylethynylene Bis-Urea Macrocycle Crystals

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Keywords: Molecular Alignment, Fluorescence Polarization, Polarization Anisotropy, Bis-Urea Macrocycle, One-Dimensional Channels

Abstract: *Bis*-urea macrocycles assemble to afford one-dimensional (1D) microchannels ~ 9 Å in diameter that have previously been shown to exhibit normal Fickian diffusion and induce selective reactivity among the confined guest molecules. Organization, especially orientation, of the guest molecules in 1D channels is a crucial factor influencing selective reactivity, birefringence, energy transfer, and electron transfer among guests. Understanding the arrangement of guest molecules in the host channel can certainly facilitate the improvement of these properties. In this study, we incorporated 5-(dimethylamino)-5'-nitro-2,2-bithiophene into well-defined columnar 1D channels located in a self-assembled structure of phenylethynylene *bis*-urea macrocycle to form a host-guest complex, and measured the orientation of the fluorescent guest confined in the channel using polarimetric fluorescence microscopy and image analysis. Guest fluorescence is shown to be polarized along the fiber axis with emission polarization values up to 0.729, indicating a high degree of orientational order within the 1D channels. The observed behavior is consistent with calculated results for the guest orientation and electronic transition dipole moment. This presentation will discuss the measurement procedures, the results from the measurements indicating the orientation of the guests, and compare the results to the computational model of the guests in the host channel.