Thermochromatism and Structural Evolution of Metastable Polydiacetylenic Crystals

Jiebin Pang, Lu Yang, Byron F. McCaughey, Huisheng Peng, Henry S. Ashbaugh, C. Jeffrey Brinker, and Yunfeng Lu

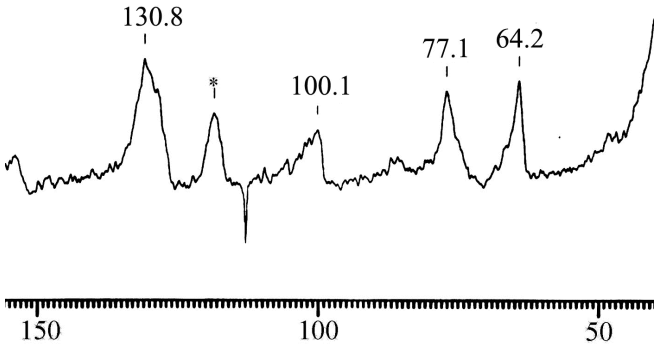

Figure SI-1. Partial ^{13}C CP/MAS NMR spectrum of the PDA–Na microcrystals polymerized by UV radiation. Asterisk indicates the spinning sideband. The presence of peak at 130.8 ppm corresponding to the sp^2 olefinic carbons of the PDA backbones suggests polymerization of the diacetylene units. The chemical shift at about 100.1 ppm can be assigned to the acetylenic carbons of the PDA backbones. The chemical shifts at 77.1 and 64.2 ppm assigned to the outer and interior acetylenic carbons in the residual unreacted monomers indicate a partial polymerization of PCDA. Estimating from the peak heights of the reacted and unreacted acetylenic carbons, the degree of polymerization is higher than 50 %.

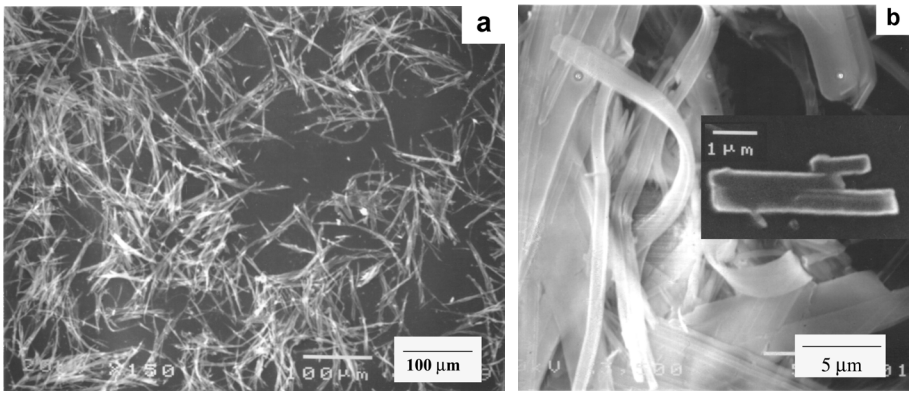

Figure SI-2. Representative SEM micrographs of the blue PDA–Na microcrystals showing a long, strip-like morphology. The inset in (b) shows an image of several small single crystals.

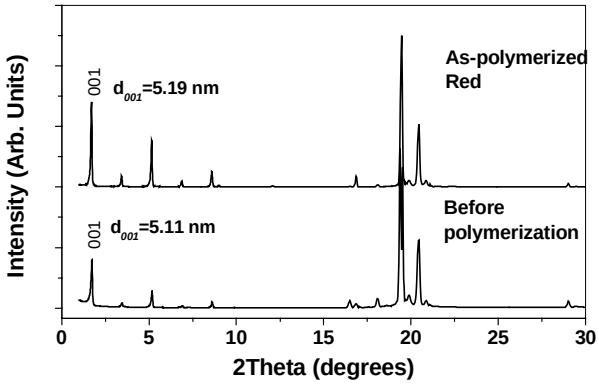

Figure SI-3. XRD patterns for the PCDA–Na microcrystals before and after topochemical polymerization. They show similar crystalline structures. Note that, however, some polymerization occurred under X-ray radiation during the scanning. This strongly supports that the molecular packing structure does not change significantly during the polymerization at room temperature.