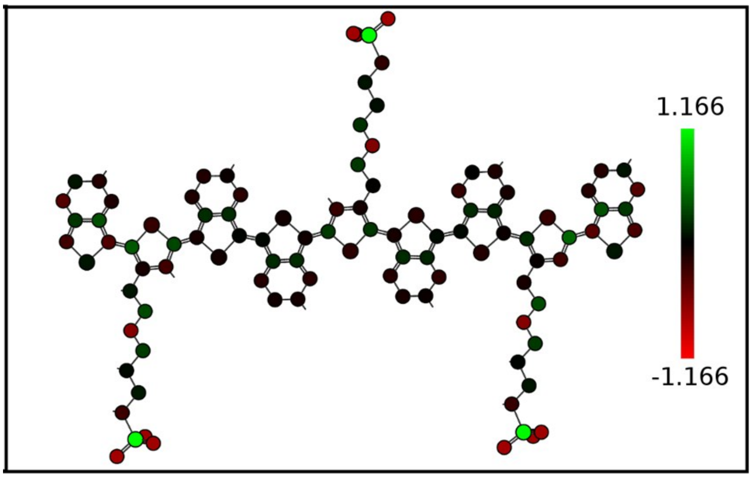
Electronic Supplementary Material (ESI) for Nanoscale.

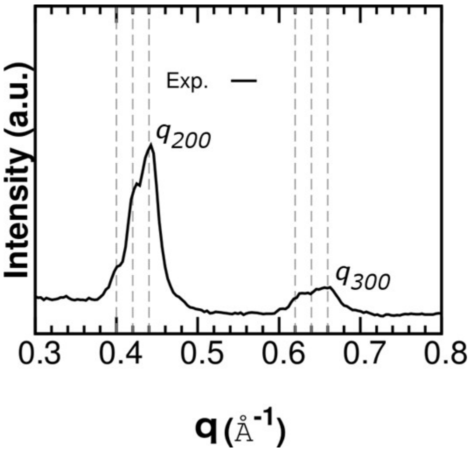
Morphology of a Self-Doped Conducting Oligomer for Green Energy Applications

Juan Felipe Franco-Gonzalez,[a] Eleni Pavlopoulou,[b] Eleni Stavrinidou,[a] Roger Gabrielsson,[a]
Daniel T. Simon,[a] Magnus Berggren[a] and Igor V. Zozoulenko[a]

[a]Laboratory of Organic Electronics, Department of Science and Technology, Linköping University, SE-601 74 Norrköping, Sweden.
[b] Bordeaux INP, Université de Bordeaux, CNRS, LCPO UMR 5629, 33600 Pessac, France.



Figures S1. Charge distribution in a ETE-S oligomer. Color bar scales show charge in units of *e*. The calculations are performed within the density-functional theory (DFT) using functional WB97XD with the 6-31+g(d) basis set as implemented in Gaussian package. The partial charge per atom were taken from the fitting to electrostatic potential (ESP) population analysis as implemented in Gaussian suite.



Figures S2. Experimental GIWAXS pattern on the oligomer film cast (the same as in Figure 2a but in an enlarged scale). A closer look shows that the 200 and 300 peaks can be deconvoluted in three peaks each, located at 0.4 Å^{-1},0.42 Å^{-1} and 0.44 Å^{-1} respectively, for 200 peak; and, 0.62 Å^{-1}, 0.64 Å^{-1} and 0.66 Å^{-1} respectively, for 300 peak. Their close vicinity and the limited resolution at the low *q*'s inhibit their deconvolution for the 100 peak. These could be suggestive of a slight disorder of the crystalline structure

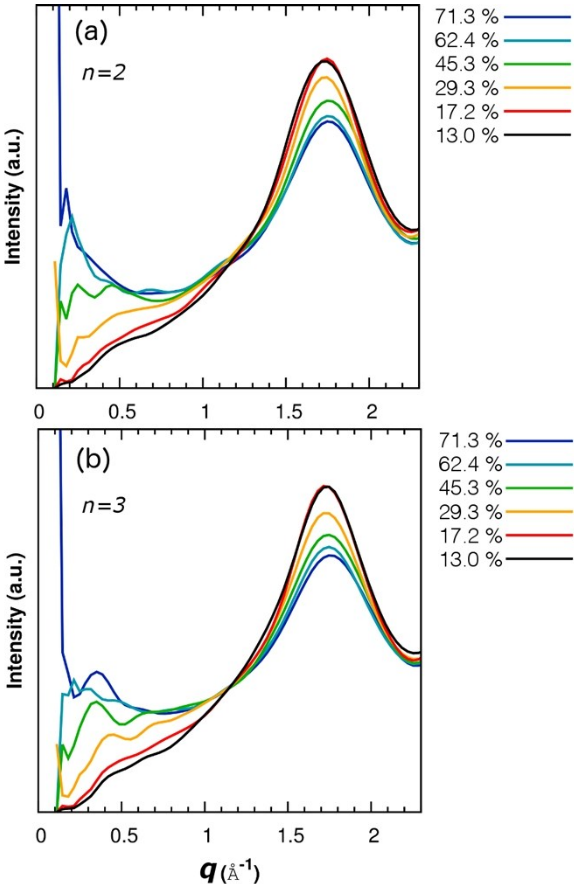


Figure S3. X-Ray Diffraction Patterns for the ETE-S oligomers with the chain lengths (a) n=2 and (b) n=3, for different water contents.