

Supporting information

**Optimizing chain alignment and preserving the pristine structure of single-
ether based PBTTT helps improve thermoelectric properties in sequentially
doped thin films**

Huiyan Zeng¹, Pablo Durand², Shubhradip Guchait¹, Laurent Herrmann¹, Céline Kiefer³,
Nicolas Leclerc^{2*} and Martin Brinkmann^{1*}

(1) Université de Strasbourg, CNRS, ICS UPR 22, F-67000 Strasbourg, France

(2) Université de Strasbourg, CNRS, ICPEES UMR 7515, F-67087 Strasbourg, France

(3) Université de Strasbourg, CNRS, IPCMS UMR 7504, F-67087 Strasbourg, France

Corresponding authors:

Nicolas Leclerc: leclercn@unistra.fr

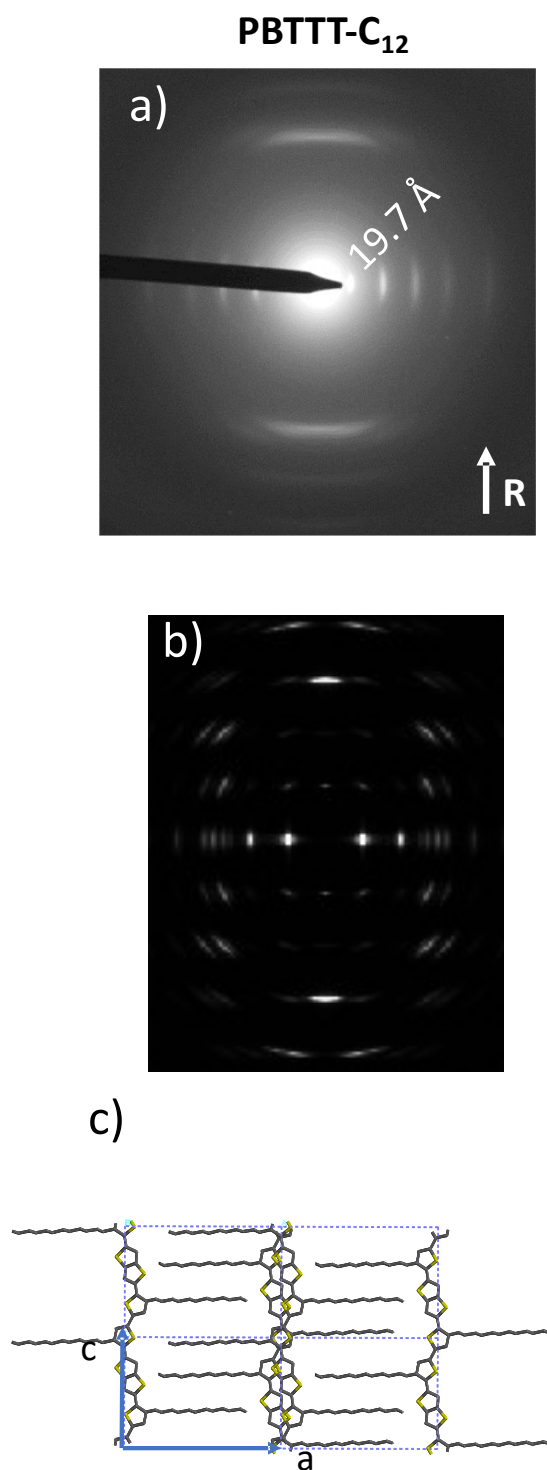


Figure S1. a) ED pattern of oriented PBTTT-C₁₂ aligned by rubbing at 125°C. b) fiber pattern calculated using Cerius² for the structural model shown in figure c) with alkyl side chains oriented perpendicular to the PBTTT backbone.

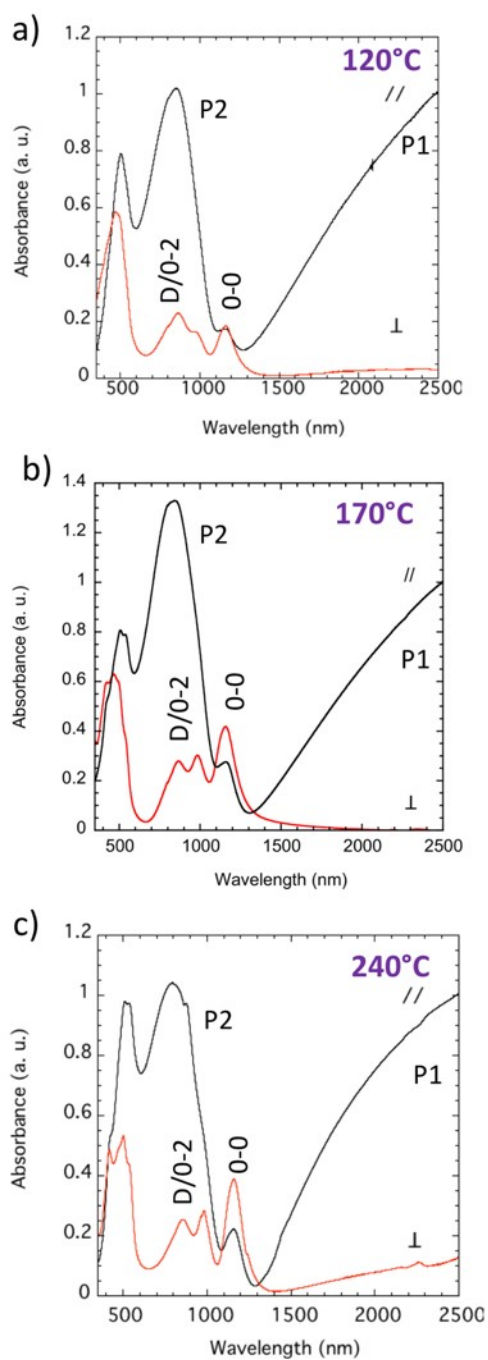


Figure S2. Evolution of the UV-vis-NIR polarized spectra of PBTTT-⁸O thin films oriented by high temperature rubbing at a) 120°C, b) 170°C and c) 240°C. The spectra are recorded for incident light oriented parallel (//) and perpendicular (red, ⊥) to the rubbing direction. The major features are annotated, including the contribution of F₆TCNNQ⁻ dimers (D) that overlaps with that of molecular F₆TCNNQ⁻.

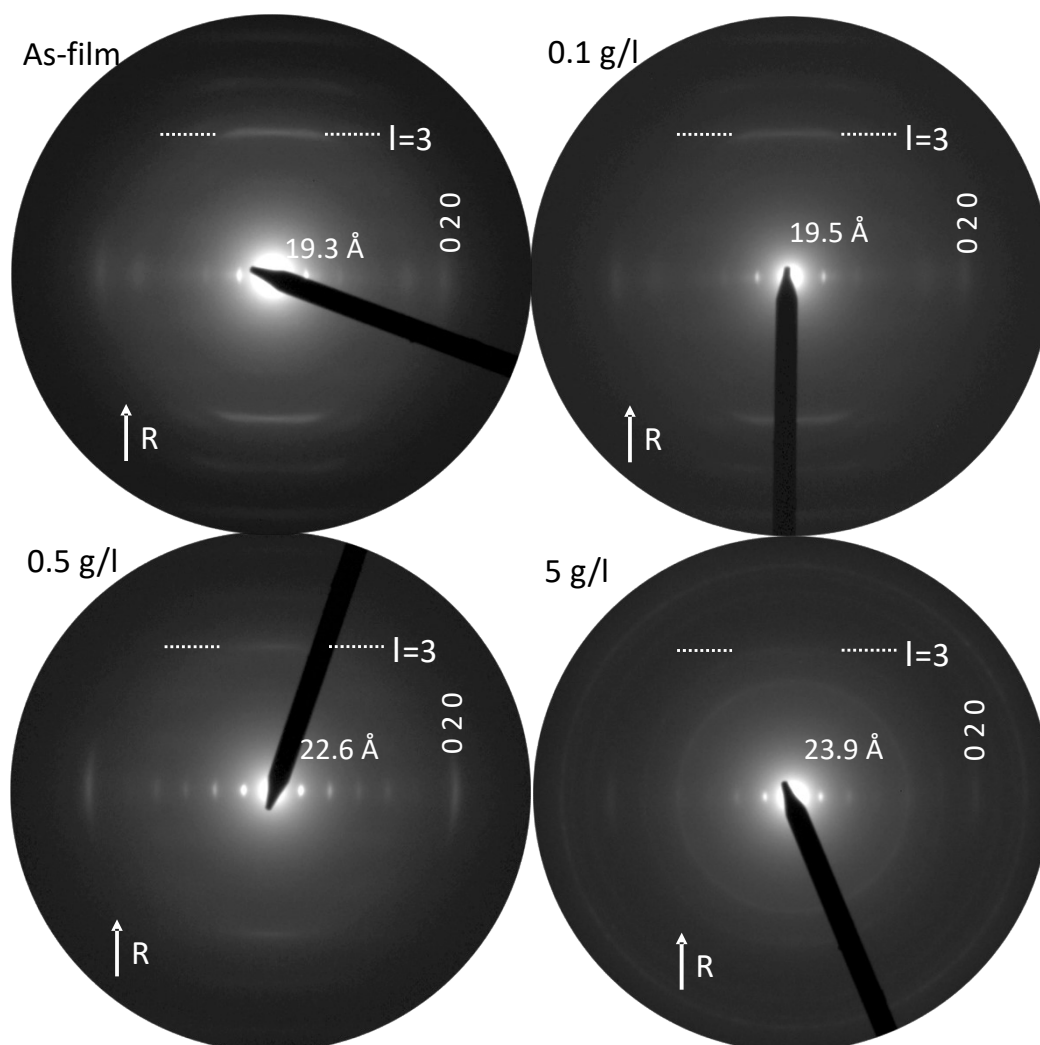


Figure S3. Evolution of the ED pattern of oriented PBTTT-⁸O rubbed at 170°C as a function of the concentration of FeCl₃ (in nitromethane). Note the fading of the meridional reflections in the $l=3$ layer line with increasing doping level. This is symptomatic of the destruction of π -stacking in individual π -stacks of PBTTT backbones upon FeCl₃ dopant intercalation. The intensity of the equatorial 0 2 0 and the h 0 0 reflections ($h=1-3$) is particularly reduced for [FeCl₃]=5g/l.

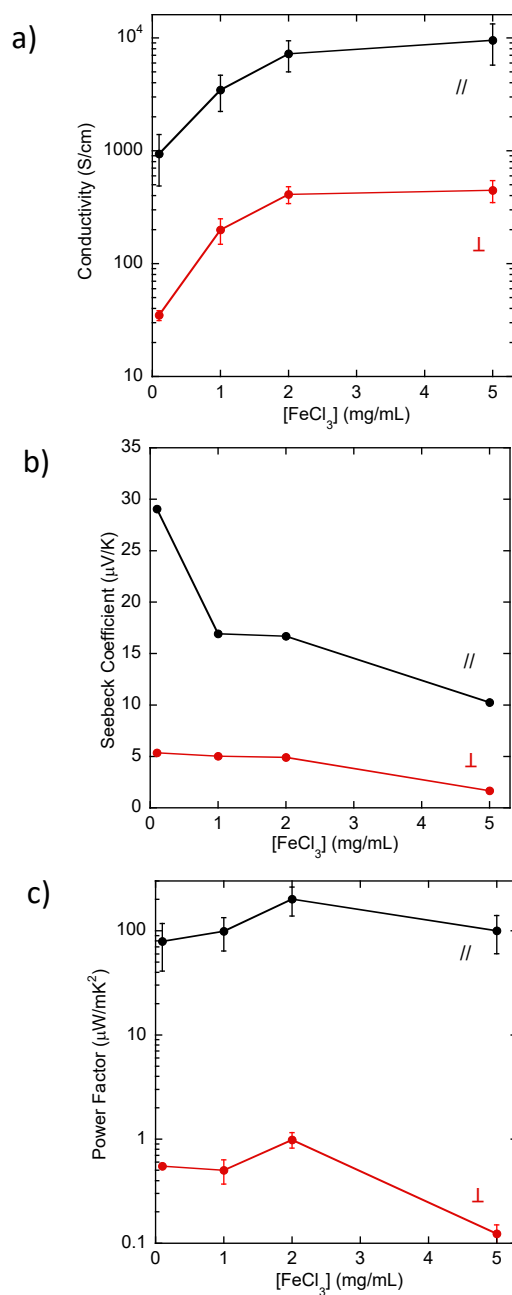


Figure S4. Evolution of the charge conductivity (a), Seebeck coefficient (b) and power factor (c) for oriented PBTtT-⁸O thin films ($T_R=170^\circ\text{C}$) doped with FeCl_3 in nitromethane for the orientation parallel (black symbols) and perpendicular (red symbols) to the rubbing direction.