

Exploring the Influence of P3HT on PTCA Crystallization and Phase Behavior in Thin Films

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Citation: To be added by editorial staff during production.

Academic Editor:

Received: date

Revised: date

Accepted: date

Published: date



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1. Results

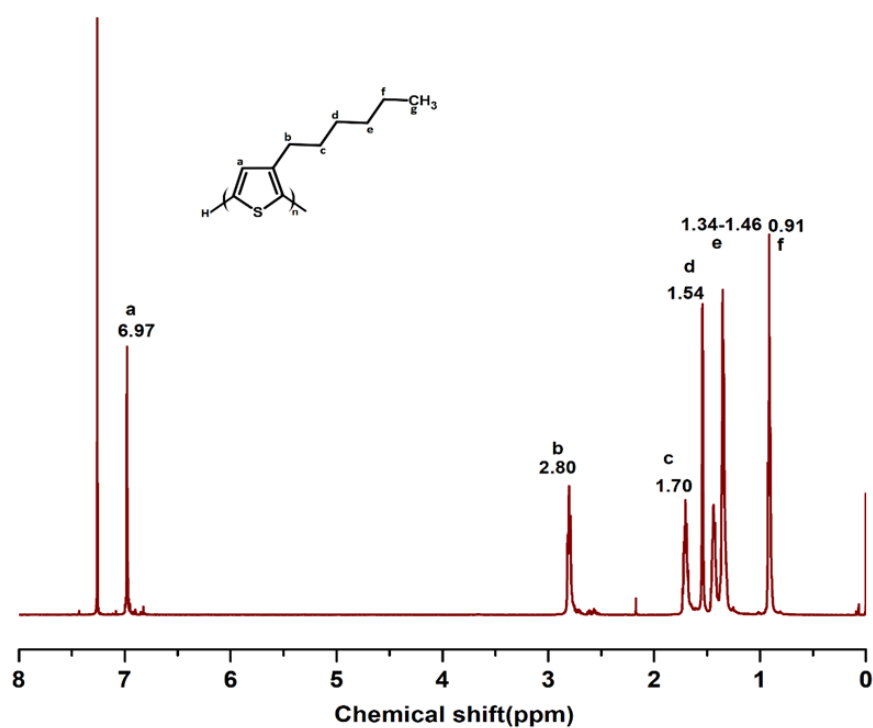


Figure S1. ^1H nuclear magnetic resonance (NMR) of P3HT.

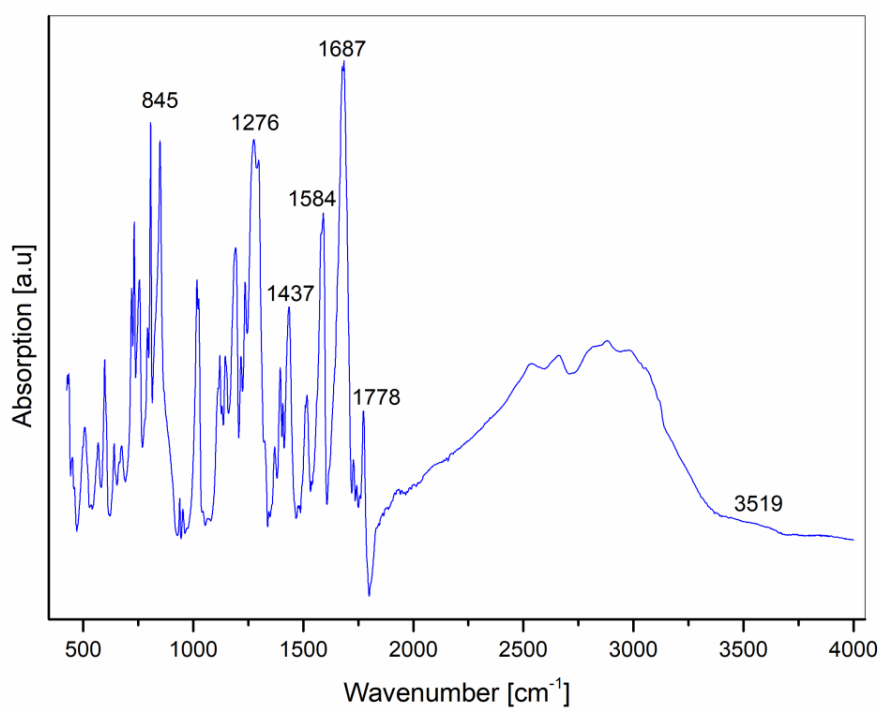


Figure S2. Fourier-transform infrared (FT-IR)–ATR of PTCA-SMs.

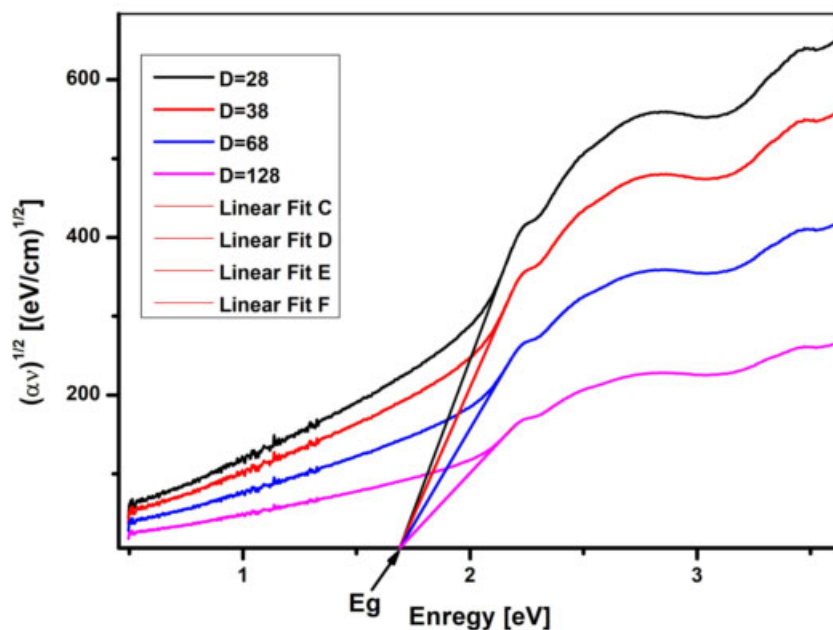


Figure S3. Energy gap of PTCA-SMs with different thickness of thin films.

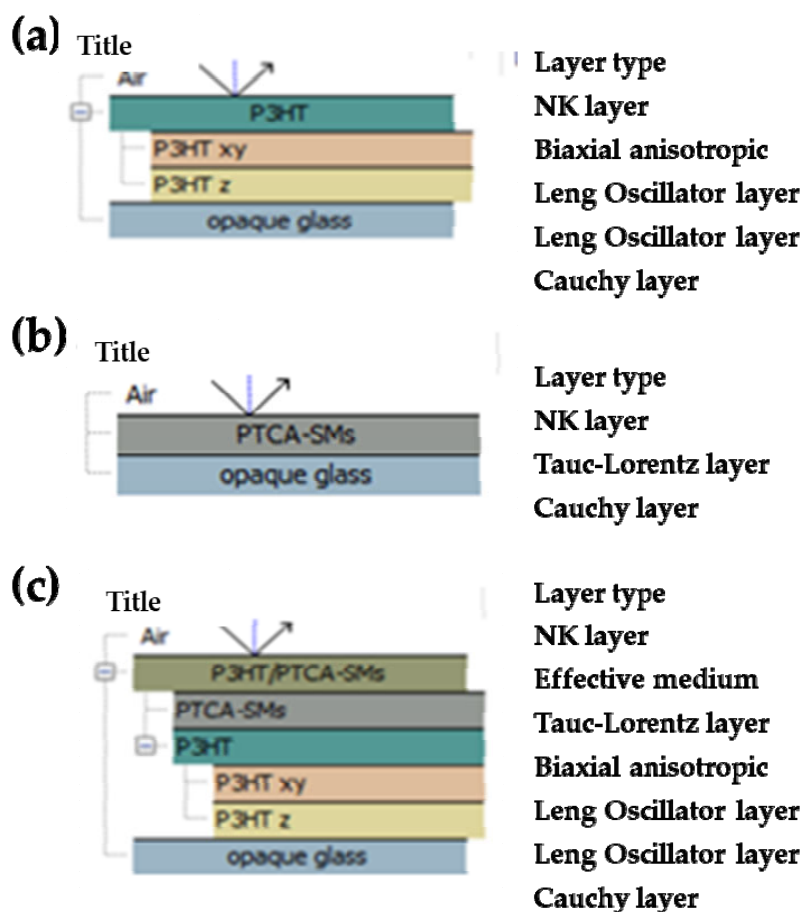
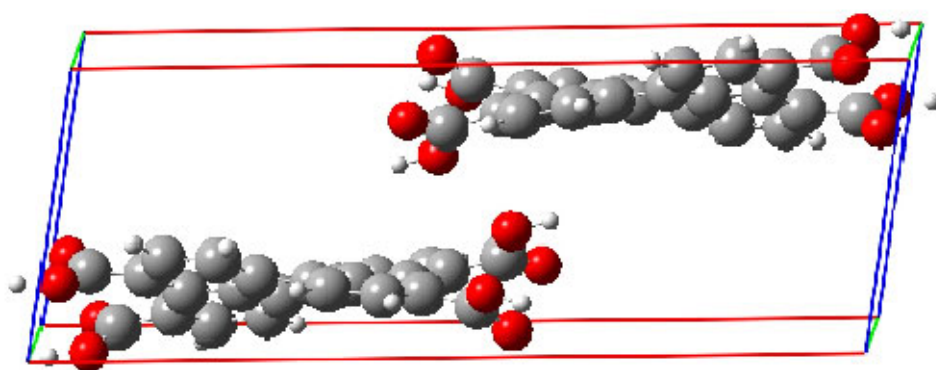
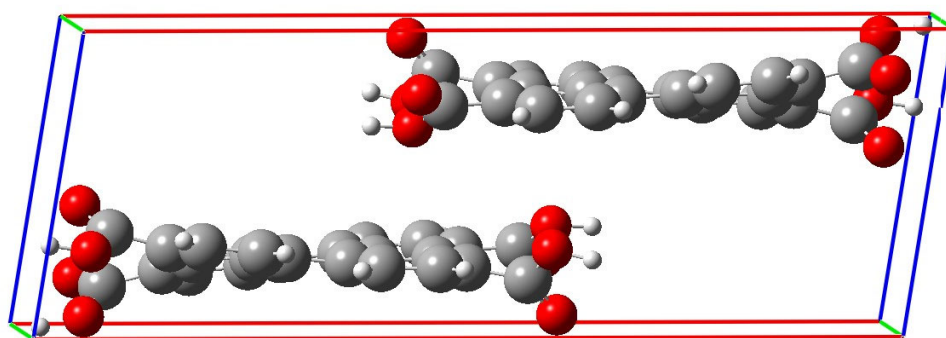


Figure S4. Ellipsometric Models of (a) P3HT, (b) PTCA-SMs, and (c) P3HT:PTCA-SMs.



a)



b)

Figure S5. Comparison of PTCA-SMs distribution in elementary cells determined based on semi-empirical calculations using (a) MOPAC2016 and matching to the X-ray pattern with (b) EXPO2014 software.

Surface roughness calculation

The root mean square roughness - R_q was applied for surface characterization of investigated samples. The R_q is defined with the following equation:

$$R_q = \sqrt{\frac{1}{m} \sum_{i=1}^m (Z_i - \bar{Z})^2}$$

where the m parameter is number of sampled points, Z_i is height of individual point and \bar{Z} is average height value [1]. R_q was determined for three surface sizes: 2×2 , 5×5 and 20×20 μm and these values are showed in graph E1 below:

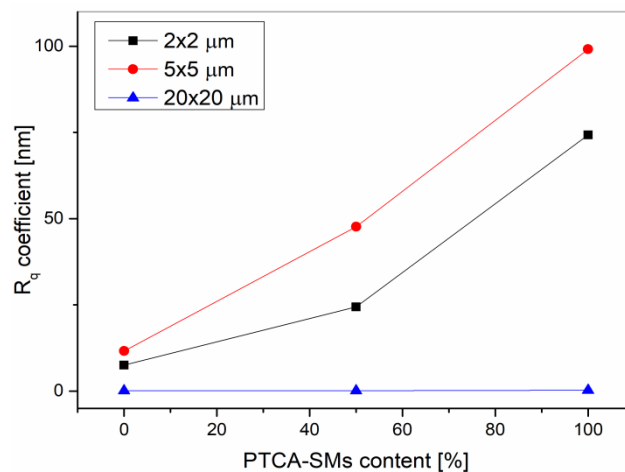


Figure S6. The mean square root of the roughness of tested samples.

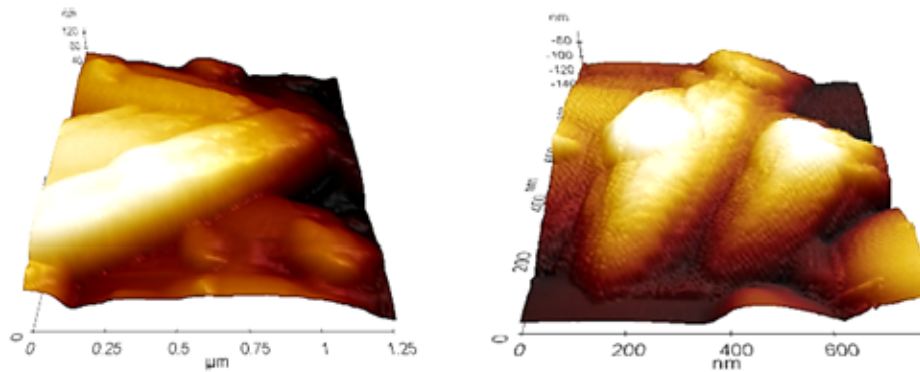


Figure S7. 1.25×1.25 and 0.7×0.7 topographic 3d images of crystallites visible in P3HT: PTCA-SMs blend surface.

References

- [1] Borgesi, A.; Tallarida, G.; Amore, G.; Cazzaniga, F.; Queirolo, F.; Alessandri, M.; Sassela, A. Influence of roughness and grain dimension on the optical functions of polycrystalline silicon films. *Thin Solid Film* **1998**, 313-314, 243–247. DOI: 10.1016/S0040-6090(97)00826-2.