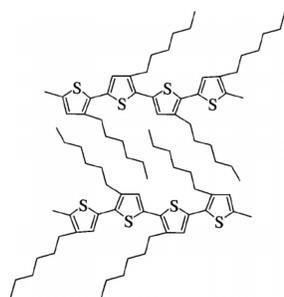


Abstract

The usual interband transitions S₀–S₀, S₀–S₁, S₀–S₂ can be clearly identified in the recently published photoluminescence measurements on P3HT layers. However, in many cases the spectra are characterized by weaker ripples besides these main features. We point out their possible interpretation by means of the H and J aggregates theory proposed by Spano [1]. Such an explanation correlates with the fact that the P3HT material in a spin-coated layer consists of the amorphous phase and one or two crystalline phases depending on the substrate surface properties.

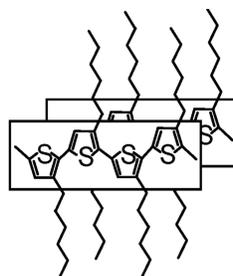
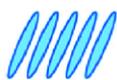
H AND J AGGREGATES

J-aggregate



- Staggered orientation
- Intrachain bonding interactions

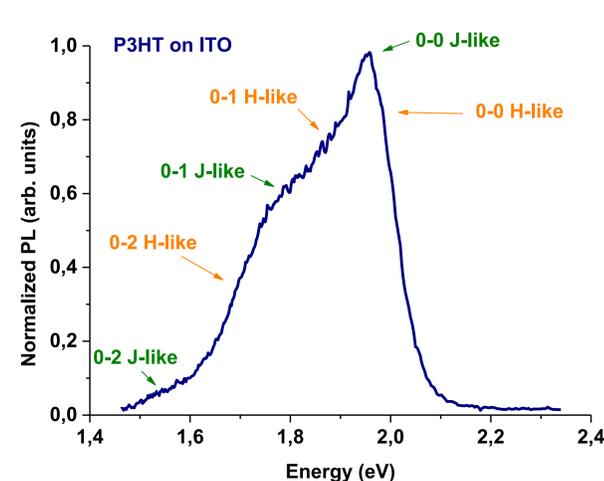
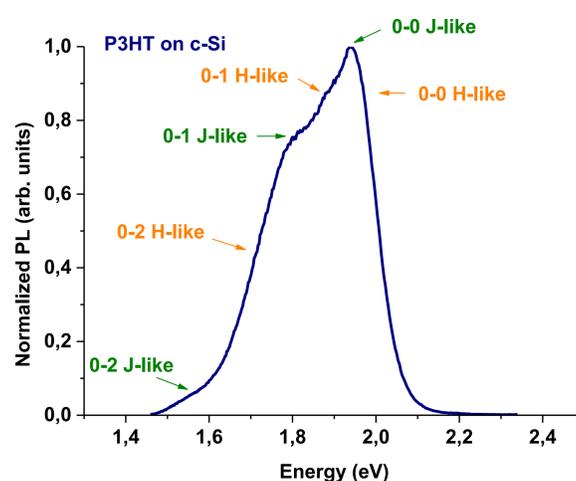
H-aggregate



- Eclipsed orientation
- Interchain Coulombic interactions

Spin coated P3HT layer – **both types** of interactions, H aggregates prevail [2, 3].

RESULTS



Photoluminescence emission spectra of P3HT layers on c-Si and ITO/glass substrates with excitation at 525 nm. The spectra are normalized to their maxima at the 0–0 vibronic transmission peaks.

- According to the Spano's calculations [4], if only H or J aggregates are in the layer the mutual distance of the spectral peaks were 1.0 – 1.2 eV. The ripples in the measured spectra are approximately as twice as closer.
- These spectral features could indicate the presence of both types of weakly interacting aggregates. One of the possible interpretations is that P3HT layer consists of pure H and J domains, respectively.
- J aggregates are typical for amorphous phases of P3HT meanwhile areas with predominant crystallinity are characteristic by interchain Coulombic interactions (H aggregates).
- The identification of H-like and J-like maxima in photoluminescence spectra of P3HT layers requires further research in the technology of samples preparation as well as numerical processing of experimental data.

LAYERS PREPARATION

Substrates

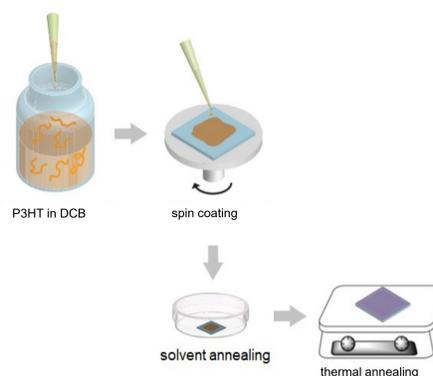
- ITO/glass substrate, RMS roughness of 6 nm
- P-type heavily doped crystalline silicon (p+ c-Si), RMS roughness below 1 nm
- cleaned using acetone and isopropanol ultrasonic bath and treated in a UV/ozone reactor for 10 minutes
- The silicon substrates etched in a 10% solution of hydrofluoric (HF) acid to remove the native silicon dioxide layer and consequently the surface was passivated in 1% HF acid solution

Spin coating

- 1.5 wt% P3HT solution in dichlorobenzene (DCB)
- Spin coating frequency: 30 rps
- Time: 45 seconds
- 110 nm thick P3HT layers
- Inert Ar atmosphere

Annealing

- solvent annealing: 20 mL for 30 min
- thermal annealing: 110 °C for 5 minutes
- Inert Ar atmosphere



MEASUREMENT

Photoluminescence

- Horiba Jobin-Yvon SPEX Fluorolog-3
- 450 W Xe lamp, Hamamatsu R928P photomultiplier tube, integration time of 0.1 s, reference Si photodiode
- Front-face (22.5°) detection, 2 nm bandpass of both double-grating monochromators
- Room temperature (300 K)
- The spectra were normalized to their maxima.

ACKNOWLEDGEMENT

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