19 a 23
JUNHO
XI
SEMANA DE PÓS-GRADUAÇÃO
EM FÍSICA DA UFPA

INSIGHTS ON P3HT PHOTO-INDUCED AGGREGATION AND OXIDATION BY ACID

Jhon R. T. Reis [1], Ruan L. S. Lima [2], Waldeci Paraguassu [3], Paulo T. Araújo[4], Newton M. Barbosa [5]

[1235] Institute of Natural Sciences, Federal University of Pará, Belém, PA, Brazil
[4]Institute of Astronomy and Physics, University of Alabama, Tuscaloosa, AL, USA
[1]jhon_etho@hotmail.com, [2]ruan_lp10@hotmail.com, [3]paraguassu@ufpa.br, [4]paulo.t.araujo@ua.edu, [5]newtonfisico@gmail.com

Resumo

The formation of organized structures in organic polymers is a well-known process, possible through various techniques, such as mixing different solvents, changing the temperature, aging the sample, and others. The resulting structures present electronic properties that differ from those of isolated polymer chains. In this study, we focus on the aggregation process of regioregular poly(3-hexylthiophene) (P3HT) induced by two different techniques. The first technique involves exposing a well-dissolved solution of P3HT in a mixture of chloroform and small quantities of methanol to a nanosecond pulsed laser centered at 532 nm, which excites within the P3HT within absorption band. The second technique involves adding a trace of hydrochloric acid to a solution of P3HT in chlorobenzene. We employed absorption spectroscopy to track the formation of P3HT aggregates. The resulting solutions in both techniques show the formation of absorption bands at around 567 nm and 603 nm. The latter band is a result of inter-chain interaction, while the former represents its vibronic progression. Additionally, bands compatible with the formation of polarons appear in the infrared portion of the spectrum. The absorption bands of the aggregates and polarons resulting from exposure to pulsed radiation increase with longer exposure times and reach an equilibrium value at 180 s. We demonstrate that by adding small concentrations of methanol (1% to 5%), the resulting solutions exhibit higher concentrations of aggregates and polarons. The ratio between the absorption band of the aggregates around 603 nm and the absorption band of the isolated chains at 450 nm varies from 0.1 in the spectrum of the solution without methanol to 0.7 in the solution containing 5% methanol. The solutions containing hydrochloric acid show an increase in the absorption bands of aggregates and polarons over time, resulting from the oxidation of the chains caused by the acid. The compatibility between the two processes indicates that exposure to pulsed radiation also oxidizes the P3HT chains, and the presence of

chloroform is crucial for this process. The results suggest that exposure to a nanosecond laser decomposes the chloroform, resulting in hydrochloric acid as a product, as previously reported for different molecules. Finally, we measure the Raman spectrum of the resulting solutions, and the results reveal that the aggregation process enhances the Raman bands of P3HT. This enhancement is a result of resonance with the excitation at 633 nm, which falls within the absorption band of the aggregates. These findings may help to understand the mechanisms behind photo-induced aggregation and optimize this technique.

Palavras chave: P3HT, Photo-Aggregation, Oxidation