PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

OXIDATIVE POLYMERIZATION OF PEDOT: INVESTIGATION OF AN UNREPORTED MECHANISM IN PEDOT:PSS SYNTHESIS

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Organic electronics is a field of materials science focused on the synthesis, characterization, design, and application of small molecules and organic polymers that exhibit electrically conductive behavior. Among the organic conducting materials, the polymer blend poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) has been widely used due to its high electrical and ionic conductivity, stability upon exposure to air, and transparency in the visible region, as well as other properties.[1] In order to maximize these advantageous properties, it is essential to synthesize PEDOT:PSS as pure as possible, with controlled chain lengths, doping levels and other parameters. This requires complete knowledge about the mechanisms of the reactions and the formation of unwanted side products. Despite the widespread use of the oxidative polymerization of the EDOT monomer in the presence of PSS, using persulfate salts as oxidizing agents,[2] the mechanism behind this synthesis method of PEDOT:PSS is still not fully understood. This gap raises questions about the possible existence of an alternative mechanism during the reaction process causing impurities that jeopardize the materials performance.[3] In fact, monitoring the oxidative polymerization of EDOT in the presence of PSS, we observe the formation of gases, which cannot be explained by the mechanism assumed to take place. In

our research, we aim to clarify the origin of this gas formation, investigate alternative mechanism and study the electrical, morphological, and optical properties of the material. For this purpose, PEDOT:PSS was synthesized by oxidative polymerization in an aqueous medium.[4] During the reaction process, gas chromatography was employed to investigate the formation of the gaseous species. To assess the material properties, polymer films were prepared by the drop-casting method for characterization. In particular, FTIR and UV–vis spectroscopy, as well as scanning electron microscopy (SEM), were performed. Complementing the UV–vis analysis, a CO/H2 sensor was used to study the possible correlation between gas formation and charge carriers. The electrical properties were determined using the four-point probe method, analyzing the effect of ethylene glycol (EG) addition. Gas chromatography result revealed the formation of carbon monoxide (CO) during the reaction, together with a further, so far unknown gas. FTIR spectroscopic analyses revealed characteristic peaks of PEDOT:PSS, while UV–vis and sensor data showed a correlation between gas release and charge carrier formation. Electrical measurements showed that EG significantly influenced the resistivity and conductance of the films. Morphological analysis indicated that, although the synthesized films exhibited good homogeneity, they displayed lower mechanical stability compared to commercial PEDOT:PSS. These results represent an initial step toward a better understanding of the processes involved in the synthesis of PEDOT:PSS and may stimulate future studies aimed at optimizing the synthetic routes and the electrical properties of the material.

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Palavras-chave: organic electronics; pedot:pss; oxidative polymerization; reaction mechanism.