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STUDY OF XRD CHARACTERISTICS OF PPy-Fe(ClO4)2 NANOPARTICLES

Chemical Science

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ABSTRACT

This work presents the synthesis of polypyrrole–iron(II) perchlorate (PPy–$Fe(ClO_4)_2$) nanoparticles using iron(III) chloride ($FeCl_3$) as the oxidizing agent. A range of monomer-to-oxidant ratios (M.R.) from 1:0.5:0.1 to 1:2:0.1, was systematically explored to assess their impact on nanoparticle formation. The resulting PPy nanoparticles were characterized by X-ray diffraction (XRD), providing key insights into their structural features and functional group behavior. The study underscores the critical role of oxidant concentration in altering the properties of PPy–$Fe(ClO_4)_2$ nanoparticles, providing valuable directions for enhancing their performance in advanced applications.

KEYWORDS

Polypyrrole, PPy, TGA, DTA, PPy-$Fe(ClO_4)_2$

INTRODUCTION

Conducting polymers have garnered considerable interest over the past few decades owing to their distinctive combination of properties, such as tunable electrical and optical behavior, mechanical robustness, straightforward synthesis, and superior environmental stability compared to conventional inorganic materials. These features have enabled conducting polymers and their composites to be widely utilized in electrical, electronic, and optoelectronic applications [1–5].

Among the various conducting polymers, polypyrrole (PPy) stands out as one of the most extensively investigated materials. PPy is appreciated for its environmental stability, facile synthesis, high electrical conductivity, and notable thermal resistance. Upon doping, its conductivity can be significantly enhanced, typically ranging between 1 and 100 $S \cdot cm^{-1}$, underscoring its unique electrical performance [6–9].

PPy has been employed in a broad spectrum of applications, including solid electrolyte capacitors, gas sensors, actuators, protective coatings, electrochromic devices, displays, polymer-based power sources, packaging, and electronic components [5–9]. Its synthesis can be achieved through two principal approaches: electrochemical polymerization and chemical oxidative polymerization, with the latter being particularly popular for producing conducting polymers due to its simplicity and versatility [9–10].

In the present study, PPy nanoparticles were synthesized via in-situ chemical oxidative polymerization using $FeCl_3$ as the oxidizing agent. The resulting product was characterized by XRD. Comparative evaluation of samples prepared with varying Fe concentrations revealed the influence of oxidant content on the structural properties of PPy–$Fe(ClO_4)_2$ nanoparticles. These findings highlight the suitability of the synthesized material for potential applications in electrical devices and sensors [11–12].

MATERIALS AND METHOD

Materials:

Analytical reagent (AR) grade pyrrole monomer (C_4H_5N) was procured from Loba Chemie Pvt. Ltd. and stored in a dark environment at 5 °C. Iron(III) chloride hexahydrate ($FeCl_3 \cdot 6H_2O$), also of AR grade, was used as the oxidant. Prior to use, pyrrole was distilled under reduced pressure to remove impurities. All solutions were prepared using deionized water.

Synthesis of PPy-$Fe(ClO_4)_2$:

A 1 M pyrrole solution was prepared in double-distilled water. The solution was continuously stirred while aqueous $FeCl_3$ was added dropwise at ~5 °C to initiate polymerization. PPy samples were synthesized with varying $FeCl_3$ concentrations. To complete the polymerization, the mixture was stirred for 3 hours. Subsequently, the dopant 0.1 M $Fe(ClO_4)_2$ was introduced as a dopant, and stirring continued for an additional 3–4 hours.

Samples were prepared with different Monomer:Oxidant:Dopant ratios (M.R.) ranging from 1:0.5:0.1 to 1:2:0.1. The reaction mixture was left undisturbed for 24 hours to ensure complete polymerization. The precipitated PPy was collected by vacuum filtration using Whatman filter paper, dried in a vacuum oven at 40–50 °C, and finely ground with a mortar and pestle for subsequent characterization.

RESULT AND ANALYSIS

The prepared sample characterized by XTD and FTIR.

X-ray Diffraction (XRD) Analysis:

The XRD pattern of PPy doped with $Fe(ClO_4)_2$ at varying molar ratios (Figure 1) reveals that the material is predominantly amorphous, as evidenced by the broad peak observed in the 20–30° region [11]. However, distinct reflections appearing between 25–30° and 45–50° suggest the presence of localized crystalline domains, likely induced by the $Fe(ClO_4)_2$ dopant. This dopant not only enhances electrical conductivity but also contributes to increased crystallinity. At lower oxidant concentrations, the formation of crystalline regions is more pronounced, whereas higher dopant levels sharpen the diffraction peaks, indicating improved structural ordering. These variations are reflected in the intensity differences across the studied ratios (1:0.5:0.1 to 1:1:0.1). Notably, the 1:0.5:0.1 sample exhibits higher overall peak intensity compared to the 1:1:0.1 sample. Such structural modifications directly influence the performance of PPy-based gas sensors, as enhanced crystallinity can lead to improved electrical conductivity and sensor efficiency.

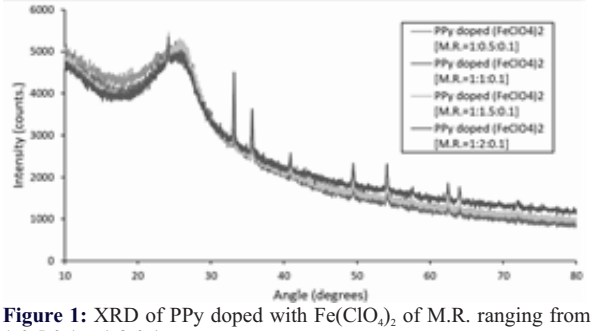

Figure 1: XRD of PPy doped with $Fe(ClO_4)_2$ of M.R. ranging from 1:0.5:0.1 to 1:2:0.1

CONCLUSION

In the present paper, we have successfully synthesized PPy-$Fe(ClO_4)_2$ nanoparticles with various concentration of Fe using chemical technique. This samples characterized by XRD. The material exhibits structural stability that strongly depends on the monomer-to-oxidant-to-dopant ratio. Some peaks at 25–30° and 45–50° indicate the presence of some crystalline areas, which is due to the $Fe(ClO_4)_2$ dopant, Optimizing these parameters is therefore essential to develop PPy materials with improved structural characteristics for applications in electronics and sensing technologies.

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