

## RESEARCH ARTICLE

# Polyaniline grafted pullulan: Optical, thermal, structural, and electrical characterization studies in combination with density functional theory calculations

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## Abstract

Polyaniline (PANI), a conducting polymer, has great interest for a large number of applications. However, poor processability and mechanical properties limits its usage and many methods like blending, grafting etc. are used to overcome this disadvantage. We have carried out grafting of PANI onto pullulan (PULL) via chemical oxidative polymerization technique. The percentage of grafting is favored by increasing concentration of aniline monomer. The formation of PANI is confirmed through UV-Vis spectroscopic studies. The possible grafting mechanism is studied using Fourier transform infrared spectroscopy and validated by Hartree-Fock density functional theory (HF-DFT) calculations. Further, thermal properties of grafted polymers are studied using differential scanning calorimetry and thermo gravimetric analysis. Using FESEM and x-ray diffraction, structural properties of graft polymer were studied. DC electrical conductivity of grafted polymer is measured from I-V characteristics, shows a significant conductivity which is the highlight of this work.

## KEYWORDS

DFT calculations, FTIR, grafting, polyaniline, pullulan

## 1 | INTRODUCTION

Polyaniline (PANI) is widely used organic conducting polymer, has significant applications in biomedical field due to its high electrical conductivity, biocompatibility, low toxicity and high environmental stability.<sup>1</sup> The conductive PANI-based nanocomposites and blends are used in the biomedical fields including antimicrobial therapy, biosensors, drug delivery, artificial muscles, nerve regeneration, neural prosthesis interfaces, scaffolds, tissue engineering, wound healing, nerve regeneration, cardiac tissue engineering etc.<sup>1,2</sup> In biomedical fields such as electrotherapy, antimicrobial

clothing, electromagnetic devices for monitoring health etc., the antimicrobial conducting PANI has been used. The PANI shows good thermal and chemical stability, pH-switching behavior, electrical and optical properties. Recently, development of PANI based ion exchange membrane for fuel cell is of interest to researchers, due to its hygroscopic nature and high proton conductivity.<sup>3</sup> While, usage is limited due to the lack of solubility in common organic solvents and film forming ability. The grafting is one of the procedures adapted to improve its processability. This allows the formation of functional groups to polymer backbone by covalent binding of a molecule.<sup>4-6</sup>