ACS APPLIED MATERIALS & INTERFACES

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Research Article

Understanding the Photochemical Properties of Polythiophene Polyelectrolyte Soft Aggregates with Sodium Dodecyl Sulfate for Antimicrobial Activity

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Cite This: *ACS Appl. Mater. Interfaces* 2021, 13, 55953−55965

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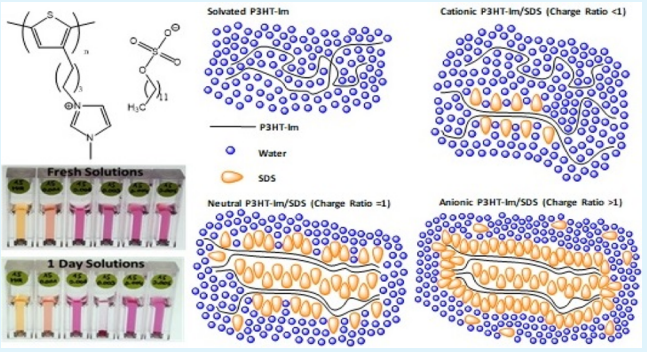
ABSTRACT: The threat of antibiotic-resistant bacteria is an ever-increasing problem in public health. In this report, we examine the photochemical properties with a proof-of-principle biocidal assay for a novel series of regio-regular imidazolium derivative poly-(3-hexylthiophene)/sodium dodecyl sulfate (P3HT-Im/SDS) materials from ultrafast sub-ps dynamics to μs generation of reactive oxygen species (ROS) and 30 min biocidal reactivity with *Escherichia coli* (*E. coli*). This broad series encompassing pure P3HT-Im to cationic, neutral, and anionic P3HT-Im/SDS materials are all interrogated by a variety of techniques to characterize the physical material structure, electronic structure, and antimicrobial activity. Our results show that SDS complexation with P3HT-Im results in aggregate materials with reduced ROS generation and light-induced anti-microbial activity. However, our characterization reveals that the presence of non-aggregated or lightly SDS-covered polymer segments is still capable of ROS generation. Full encapsulation of the P3HT-Im polymer completely deactivates the light killing pathway. High SDS concentrations, near and above critical micelle concentration, further deactivate all anti-microbial activity (light and dark) even though the P3HT-Im regains its electronic properties to generate ROS.



KEYWORDS: *reactive oxygen species (ROS), poly-(3-hexylthiophene) (P3HT), imidazolium, sodium dodecyl sulfate (SDS), Escherichia coli (E. coli), ultraviolet visible irradiation and polymer aggregate material*

INTRODUCTION

Bacterial resistance to traditional small-molecule antibiotic treatments is an ever-increasing problem in today's world.[1−3] The rapid increase is attributable to the slow development of novel antimicrobial agents and the rapid evolution of bacteria. Bacteria are known to have many defense systems against antibiotics that enable the bacteria to modify drug protein targets,[4,5] generate neutralization agents for known antibiotics,[6,7] or adapt protein efflux pumps[8−10] to quickly remove the antibiotic from within the cell envelope. This has led scientists to look for new alternative anti-bacterial strategies. A broad range of therapies (*ex situ* contact killing,[11−13] photodynamic therapy (PDT),[14−16] and targeted radiotherapies)[17,18] are being explored as alternative anti-bacterial strategies for their ability to trigger bacterial death through non-specific cell killing pathways.

In the PDT, water-soluble, metal-free conjugated polyelectrolytes are an emerging field of interest. For example, water-soluble porphyrin oligomers,[19,20] push−pull donor−acceptor conjugated polymers,[21−23] and polythiophene-conjugated polymer derivatives[24,25] exhibit many attractive properties for PDT and anti-bacterial therapies due to their large absorbance cross-sections, fluorescence, and sensitizing abilities, especially in the production of reactive oxygen species (ROS) including peroxides, singlet oxygen, and hydroxyl radicals. Most importantly, "push−pull" donor−acceptor and polythiophene-conjugated polymers are solution processable, easily tunable material platforms for bacterial targets by modification of side functional groups or incorporation into block copolymers.[23]

Synthetic functional group modifications pendant to the backbone of conjugated polyelectrolytes (specifically polythiophenes) can be used to tune the electronic properties and

Received: September 25, 2021
Accepted: November 3, 2021
Published: November 17, 2021