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Self-Exfoliated COF Encapsulate Bacteria and Fungi via Electrostatic Interaction: A Potential Broad-Spectrum Contact-Killing Strategy

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Abstract. Microbial contamination by bacteria and fungi poses a serious threat to global public health security. With the widespread dissemination of drug-resistant strains and the high energy consumption and toxic residues associated with traditional disinfection methods, there is an urgent need to develop novel, efficient, and residue-free broad-spectrum antimicrobial strategies. Herein, we synthesized a cationic β-ketoenamine-linked covalent organic framework, EB-TFP-COF. The material exhibits high crystallinity, excellent water stability, strong visible-light absorption, and rapid self-exfoliation capability in water. Self-exfoliated EB-TFP-COF uses electrostatic interactions to encapsulate E. coli and yeast effectively, leveraging the positive charge of its backbone to form a uniform core-shell structure. The formation of the encapsulation layer was confirmed by PXRD and confocal microscopy. This study establishes a COF-based encapsulation platform for bacteria and fungi, providing a foundation for broad-spectrum contact-based antimicrobial strategies and offering new insights for designing COF-based antimicrobial materials.

Keywords: Covalent organic frameworks, Self-exfoliation, EB-TFP-COF, Electrostatic encapsulation, Contact-killing

1. Introduction

Serious threats to global public health security are posed by bacterial and fungal contamination, particularly with regard to food safety, medical device coatings and water treatment systems [1]. Pathogenic bacteria such as Escherichia coli [2] (Gram-negative bacteria), Staphylococcus aureus [3] (Gram-positive bacteria), and Candida albicans [4] (fungus) can develop persistent resistance to antibiotics and may form biofilms, making them difficult to treat and leading to persistent infections and health crises. As antimicrobial resistance becomes more severe, the drawbacks of traditional disinfection methods (such as oxidative disinfection, irradiation, and antibiotic therapy) have also become apparent [5]. Therefore, there is an urgent need for the development of novel, highly effective, broad-spectrum antimicrobial strategies.

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Covalent organic frameworks (COFs) are built from organic units linked by robust covalent bonds, offering abundant surface groups, adjustable pores, and good biocompatibility [6]. These features have driven their exploration in areas like gas adsorption, catalysis, sensing, and biomedicine [7]. Among the different linkage types, β-ketoenamine COFs stand out because they combine structural stability with a distinct bonding mechanism [8]. When the COF carries positive charges, it forms strong electrostatic interactions with negatively charged microbial membranes, thereby establishing a critical structural foundation for contact sterilization. Additionally, its conjugated structure boosts light absorption and charge separation [9], delivering strong photothermal and photodynamic effects under light. All this makes β-ketoenamine COFs compelling options for photo-responsive antibacterial applications.

Aside from carrying antimicrobial agents such as AgNPs [10] or Cu_2O [11], COFs can interact directly with microbial cells via surface encapsulation. In the single-cell nanoencapsulation approach, a core-shell structure is formed around individual cells by either in situ growth or self-assembly of a COF shell [12]. When that shell carries positive charges, it naturally binds to the negatively charged cell membrane via electrostatic interactions, delivering a contact-killing effect. This mechanism does not rely on added photosensitizers or ion release, so it comes with perks in terms of biosafety and a lower risk of driving antibiotic resistance [13]. However, systematic work on how COFs encapsulate microbes and what that means for their antimicrobial performance is still limited.

Here, we show that both E. coli and Yeast can be directly wrapped in a uniform EB-TFP-COF shell thanks to electrostatic interactions that drive the assembly process. This encapsulation strategy offers a straightforward, contact-based route to microbial inhibition and could serve as a versatile platform for designing new antimicrobial materials. By establishing a well-defined COF coating method that works for bacteria and fungi alike, the work sets the stage for deeper mechanistic studies into contact killing and opens up fresh directions for advanced antibacterial design.

2. Synthesis and characterization of EB-TFP-COF

EB-TFP-COF was synthesized solvothermally following a reported procedure [14]. Its crystalline structure was confirmed by powder X-ray diffraction (PXRD) , which showed a strong reflection (100) at $2\theta = 3.3°$ and a broad peak (001) near 27° (Fig. 1a). Fourier Transform infrared (FTIR) spectroscopy revealed the disappearance of the N-H stretching bands of EB (3191 and 3313 cm-1) and the aldehyde C-H stretching band of TFP (O=C-H, at 2894 cm-1), as well as new C=C stretching vibrations at 1585 cm-1, confirming the formation of EB-TFP-COF (Fig. 1b). N_2 adsorption-desorption measurements gave a type I isotherm, characteristic of microporous materials, with a BET surface area of 920.1 m^2/g (Fig. 1c) and a pore size of 1.72 nm (Fig. 1d), indicating the successful synthesis of EB-TFP-COF with high specific surface area.

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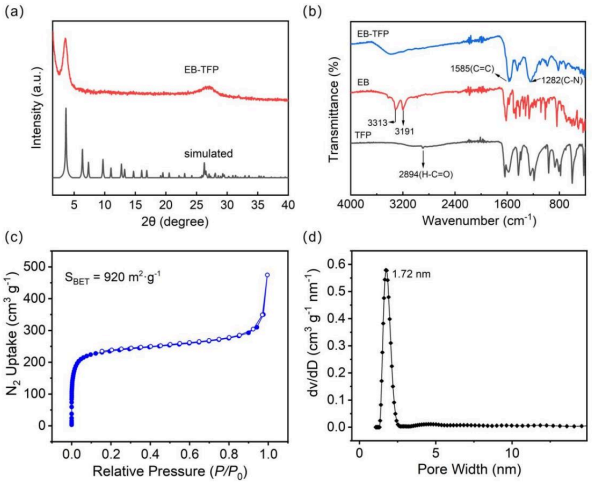

Figure 1. (a) PXRD patterns and (b) FTIR spectra of EB-TFP-COF. (c) The nitrogen sorption isotherm profiles measured at 77 K and (d) the pore size distribution profiles of EB-TFP-COF

3. Self-exfoliation of EB-TFP-COF

The morphology of EB-TFP-COF was examined by SEM, which revealed an irregular multilayered stacking structure (Fig. 2a). After stirring in water for 2 h, EB-TFP-COF underwent self-exfoliation (Fig. 2b). Comparison of the PXRD patterns before and after self-exfoliation showed that the diffraction peaks at 3.3° and 27° remained observable, confirming the occurrence of self-exfoliation (Fig. 2c). Solid-state UV–vis diffuse reflectance spectroscopy (DRS) demonstrated that EB-TFP-COF exhibits strong absorption in the range of 400–600 nm (Fig. 2d), and the optical bandgap (Eg) is determined to be 2.08 eV via Tauc plot analysis (inset of Fig. 2d), demonstrating its potential for photo-responsive antibacterial applications.

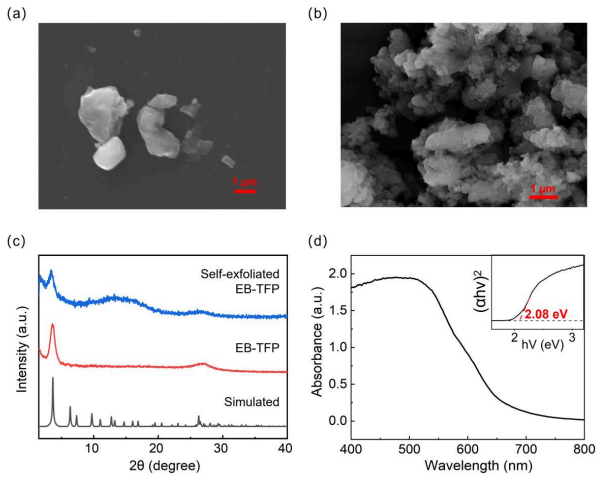

Figure 2. SEM image of (a) EB-TFP-COF and (b) Self-exfoliated EB-TFP-COF.(c) PXRD patterns of EB-TFP-COF before and after self-exfoliation. (d) UV–vis DRS and Tauc plot (inset) of EB-TFP-COF

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4. EB-TFP-COF-encapsulated microbial system

To evaluate the water stability of EB-TFP-COF for aqueous-phase applications, the material was immersed in ultrapure water for 7 days. As shown in Fig. 3a, the PXRD pattern remained unchanged, indicating its excellent water stability. Electrostatic adsorption between EB-TFP-COF and E. coli requires distinct surface charge characteristics. Zeta potential measurements revealed that EB-TFP-COF is positively charged within the pH range suitable for E. coli survival (pH 6.0–8.0), while E. coli exhibits a negative surface charge (Fig. 3b). E. coli cells in the logarithmic growth phase were collected and incubated with self-exfoliated EB-TFP-COF under stirring. The PXRD pattern of the resulting EB-TFP/E. coli assembly displayed characteristic diffraction peaks at 3.3° and 27° (Fig. 3c), confirming the electrostatic adsorption and successful binding between EB-TFP-COF and E. coli. Confocal laser scanning microscopy (CLSM) images revealed that EB-TFP-COF formed a uniform encapsulation layer on the surfaces of both E. coli (Fig. 4a) and Yeast (Fig. 4b) , a morphological feature that provides a structural foundation for its further application in broad-spectrum contact-killing antibacterial strategies.

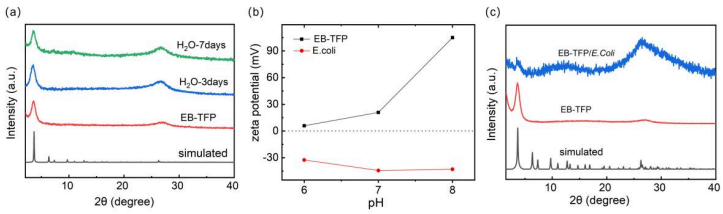

Figure 3. (a) PXRD patterns of EB-TFP-COF after immersion in water for 3 and 7 days. (b) Zeta potential measurements of EB-TFP-COF and E. coli (c) PXRD patterns of EB-TFP-COF after encapsulation of E. coli

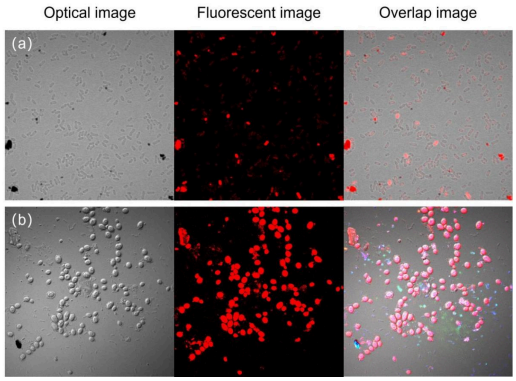

Figure 4. CLSM image of (a) E. coli and (b) Yeast encapsulated in EB-TFP-COF

5. Conclusion

We have developed an encapsulation system based on a cationic β-ketoenamine COF. EB-TFP-COF exhibits high crystallinity, strong visible-light absorption, excellent water stability, and rapid self-exfoliation capability. Leveraging its intrinsic positive charge, EB-TFP-COF successfully encapsulates E. coli and Yeast via electrostatic interactions, forming uniform core–shell structures. This study establishes a COF encapsulation platform for both bacteria and fungi. This lays the structural foundation for the development of broad-spectrum, contact-based antimicrobial strategies, opening up new possibilities for the design of advanced COF antimicrobial materials.

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