SUPPORTING INFORMATION

Crystallization ripening and erosion of calcium oxalate under the effect of bacteria and polymer materials surface

Xiran Shen‡[ab], Wentao Chen‡[c], Li Guo[a], Huayu Li[d], Hong Chen[c], Fan Liu*[e]*

[a] Research School of Polymeric Materials, School of Material Science & Engineering, Jiangsu University, Zhenjiang, 202113, China

[b] Jiangsu Biosurf Biotech Co., Ltd, Suzhou, 215123, P. R. China.

[c] State and Local Joint Engineering Laboratory for Novel Functional Polymeric Materials, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou, 215123, China

[d] Material and Analytical Sciences, Boehringer Ingelheim Pharmaceutical Inc., Ridgefield, CT 06877, United States

[e] Jiangsu Key Laboratory of Neuropsychiatric Diseases, Jiangsu Province Engineering Research Center of Precision Diagnostics and Therapeutics Development, and College of Pharmaceutical Sciences, Soochow University, Suzhou, 215123, China

‡ These authors contributed equally to this work.

* Corresponding authors

1. Experimental Procedures

1.1 Preparation of crystal culture solution

The supersaturation of calcium oxalate in solution C1 is 2.08, and in C2, it is 8.09. Solution C1 is formulated with a Ca2+ to Ox2- ratio of 5.75:0.33, while solution C2 has a Ca^{2+} to Ox^{2-} ratio of 10:1. Taking C1 as an example, the process is as follows: $CaCl_2$ (0.638 g, 5.75 mmol) was dissolved in deionized water (250 mL). An *E. coli* solution (10^7 CFU/mL, 2 mL) was added to the solution at the sterile bench. After the solution stabilized, 250 mL of $Na_2C_2O_4$ (0.043 g, 0.336 mmol) solution was added, and the mixture was left to observe precipitation. The same process was repeated for *S. aureus*, inhibitors, etc.

1.2 Treatment of bacteria

E. coli (MG1655) frozen at -80°C were screened on LB plates. They were incubated at 37°C for 12 hours to achieve activation. The activated individual colonies were added to 2 mL of LB liquid medium and incubated at 37°C and 190 rpm in a shaker for 8-12 hours. *S. aureus* (ATCC-6538) were cultured in broth medium for 12−18 h. After diluting the bacteria with sterilized phosphate buffered saline (PBS) buffer, the OD of the bacterial solutions were tested at 600 nm (*E. coli* MG1655) and 670 nm (*S. aureus* ATCC-6538). The density of the bacterial suspensions were reduced to 10^7 CFU/mL.

1.3 Synthesis of Polyurethane (PU)

The polyurethane resin (10 g) was dissolved in anhydrous ethanol (90 g) with the addition of benzophenone 0.65 g. After complete dissolution, the coating solution was poured onto a Petri dish and baked in an oven at 60°C for 3 hrs. After molding, it was cured under UV for 2-3 minutes.

1.4 Preparation of PU-PNBB

The above PU coating solution was uniformly mixed with PNBB (1 mg/mL) dissolved in anhydrous ethanol at 5% solids before drying. The remaining steps are consistent with PU.

2. Results and Discussion

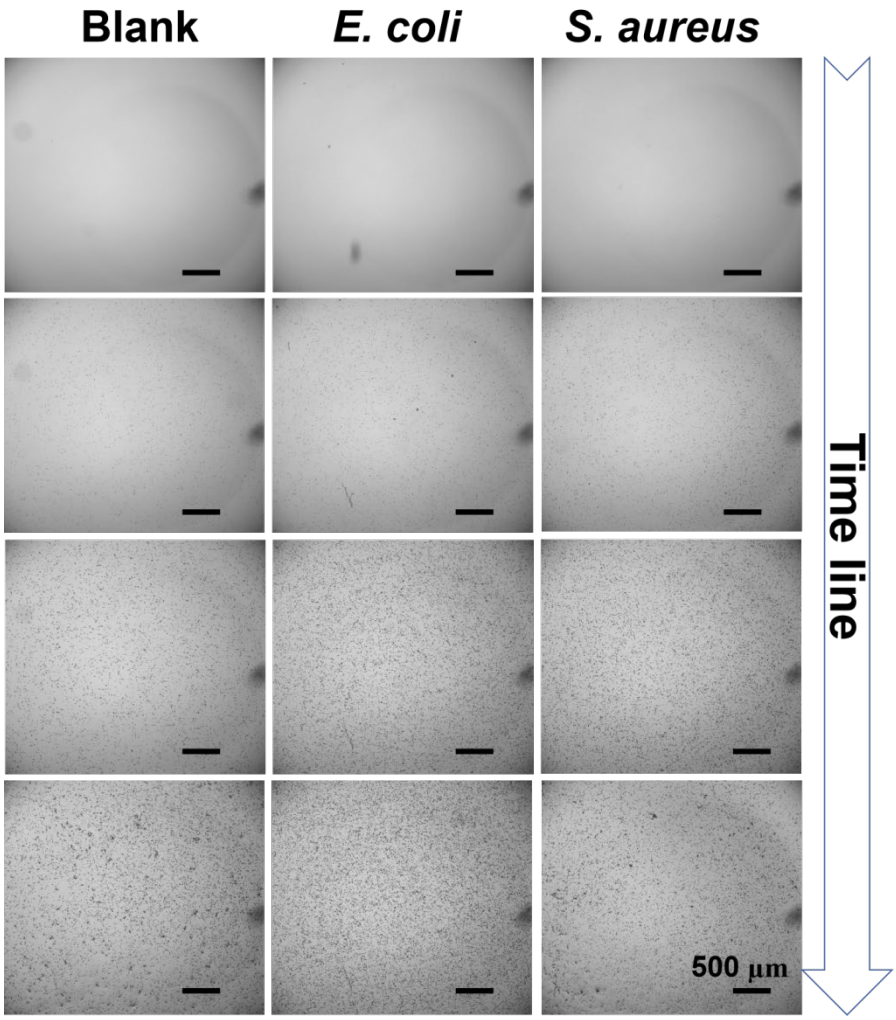

Fig. S1 Images of calcium oxalate crystals captured using a crystallization monitoring system (PCM) were incubated with or without bacteria at room temperature.

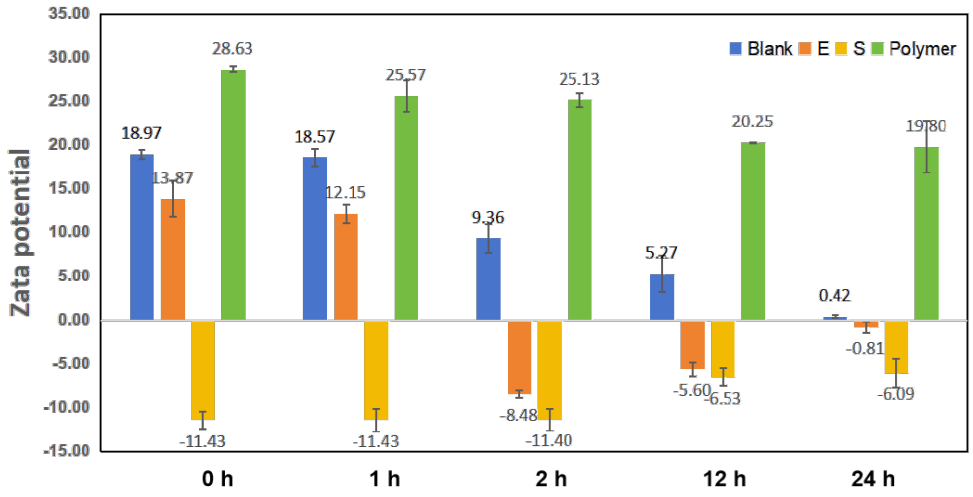

Fig. S2 Zeta potential of different growth solutions at different times.

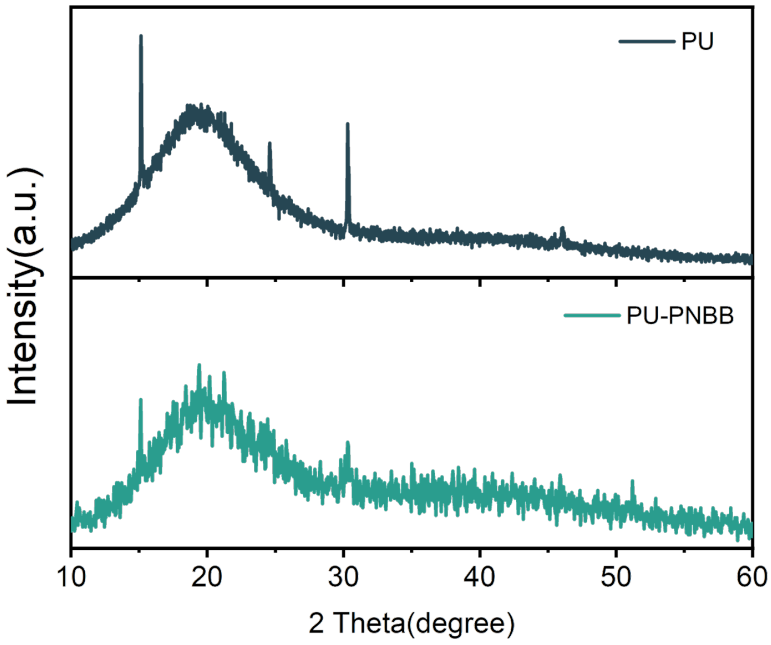

Fig. S3 PXRD spectra of PU and PU-PNBB surfaces.

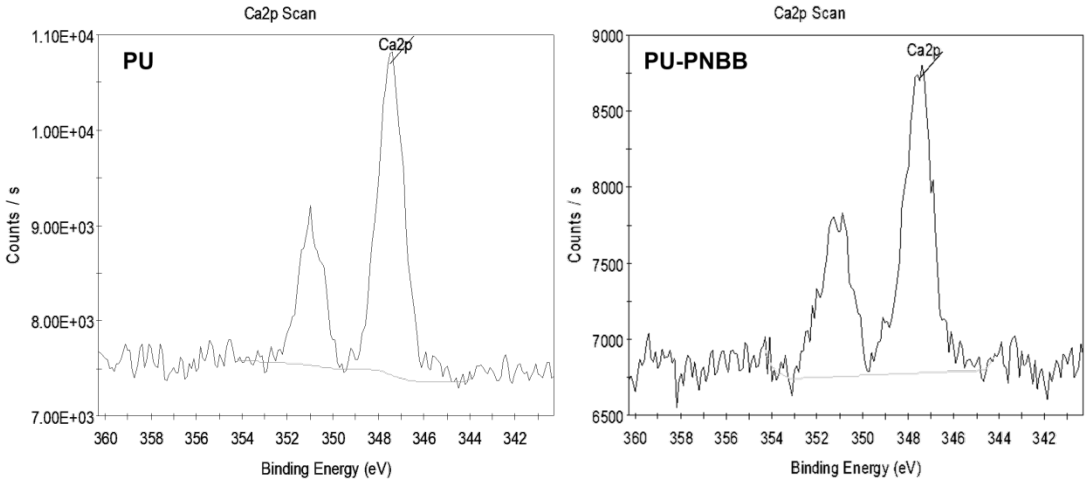

Fig. S4 XPS spectra of PU and PU-PNBB surfaces.

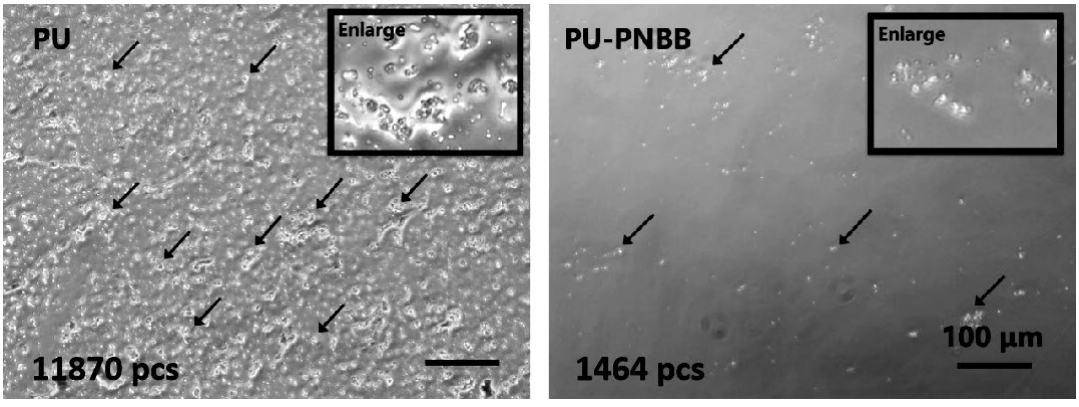

Fig. S5 Microscopic images of PU and PU-PNBB films immersed in artificial urine for 15 days.

In the X-ray powder diffraction (PXRD) analysis of the modified polyurethane (PU-PNBB) surfaces, the uneven baseline shown in **Fig. S3** primarily originates from the inherent amorphous nature of PU. Despite the uneven baseline, the distinct diffraction peaks confirm that the modification of PU-PNBB did not alter the crystal structure, consistent with the observations made using microscopy in **Fig. S5** and **S1**. Furthermore, the reduction in the number of crystals led to decreased intensity of the diffraction peaks, indicating that the modified PU-PNBB significantly inhibits the growth of calcium oxalate crystals. This finding highlights the potential application of modified polyurethane surfaces in inhibiting the formation of calcium oxalate crystals and validates their effectiveness as crystal growth inhibitors. Elemental analysis using X-ray Photoelectron Spectroscopy (XPS) revealed that the calcium concentration on the surface of PU-PNBB is significantly lower than that on the surface of PU, indicating a reduction in the number of crystals. This further corroborates the inhibitory effect of PU-PNBB (**Fig. S4**).

Tab. S1 Distribution of D10, D50, and D90 of CaOx crystals in the early, middle, and late stages in solutions with different components.

	Early stage（μm）			**Mid stage（μm）**			**Late stage（μm）**		
	D10	D50	D90	D10	D50	D90	D10	D50	D90
Blank	4.19	5.17	8.98	9.68	14.35	22.08	12.57	22.43	37.12
S.×1	4.32	5.36	6.67	7.69	10.41	13.57	10.56	15.88	24.08
S.×3	4.52	5.43	6.76	8.07	11.83	17.72	9.93	16.86	27.73
E.×1	4.47	5.38	6.13	8.22	10.99	16.88	9.61	15.28	23.63
E.×3	6.28	8.93	10.06	9.48	15.59	26.08	12.28	23.27	39.23