Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information For

Phosphorylation of collagen fibrils enhances intrafibrillar mineralization and dentin remineralization

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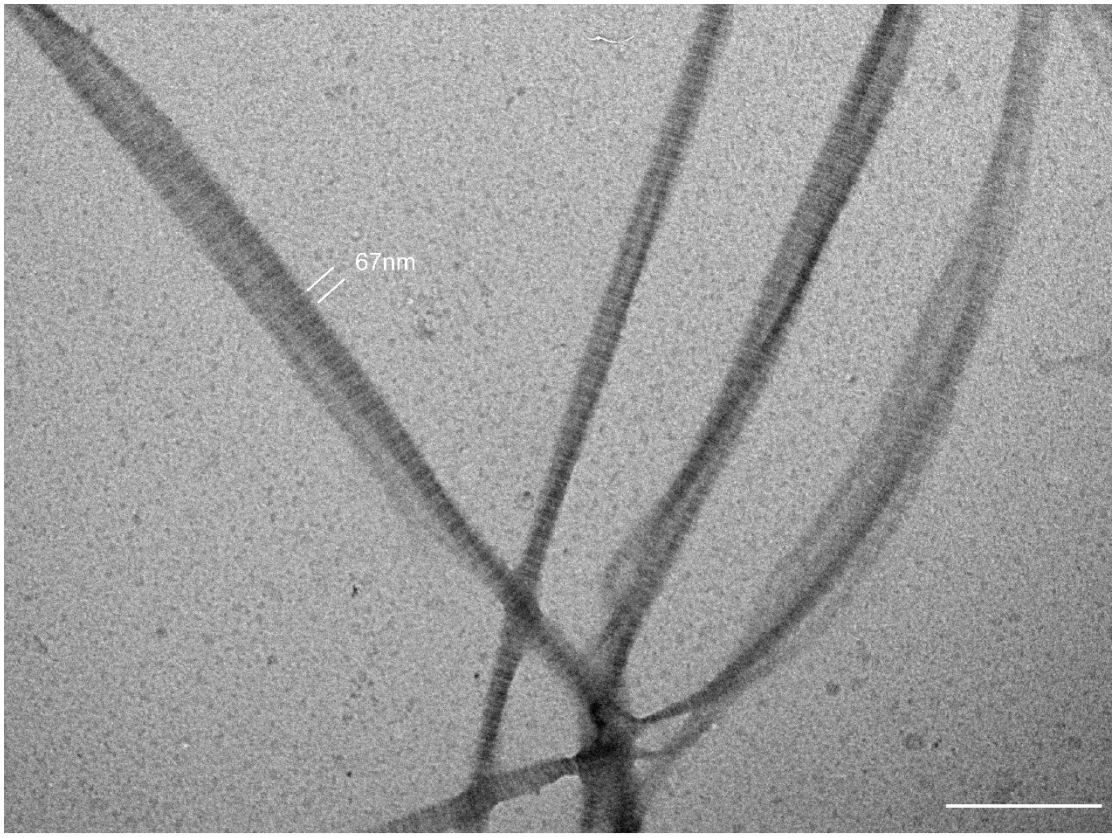
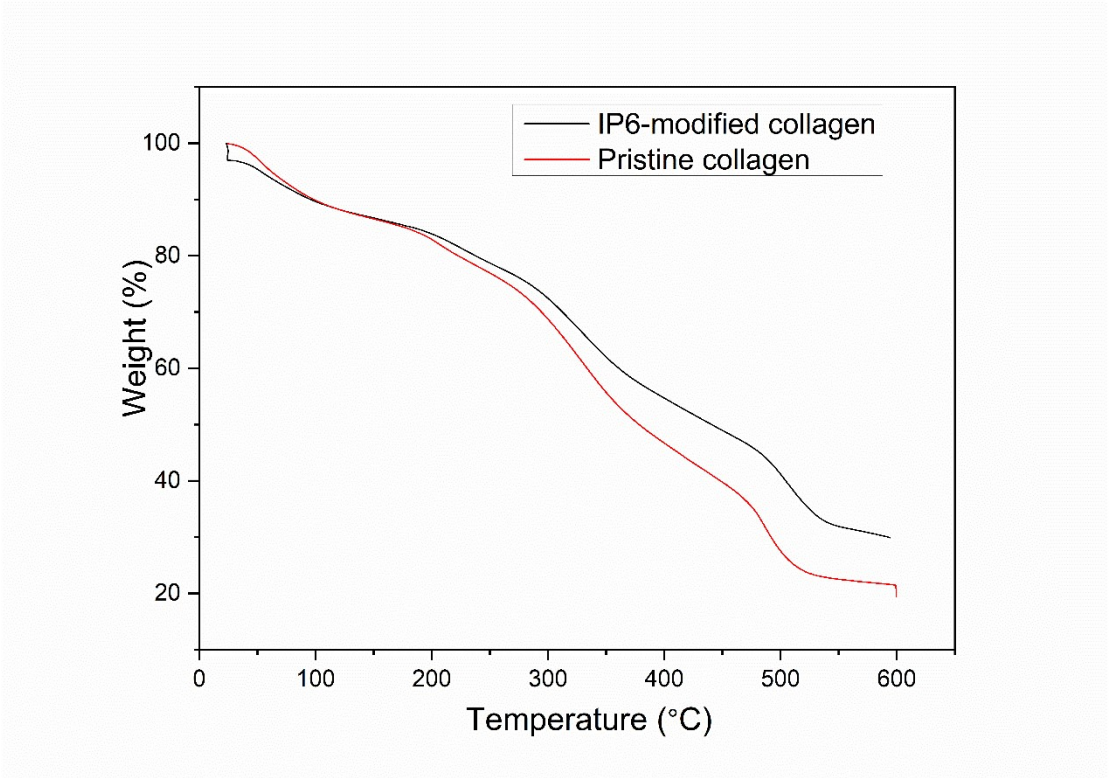
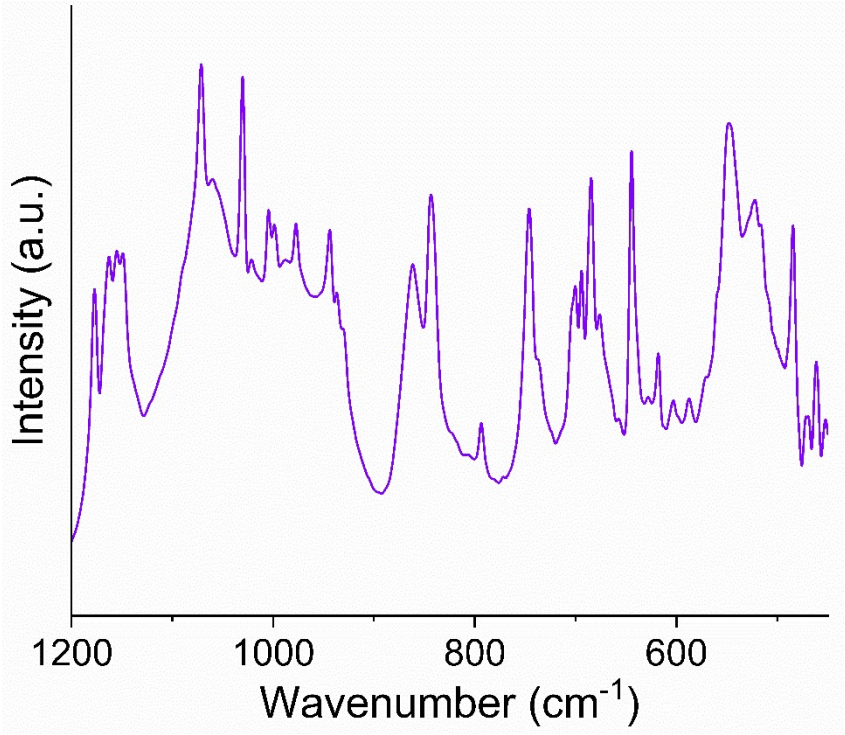
Supported Figures



Figue S1. TEM images of self-assembled collagen fibrils with a typical 67 nm D-band structure. Scale bar: 500 nm.



Figue S2. The representive curves of the TGA of pristine collagen and IP6-modified collagen after 4-day mineralization.



Figue S3. FTIR spectrum of IP6.

Supported Text

1. Calculation of interaction energy between IP6 and collagen fibrils

The fitted adsorption curves of IP6 on collagen fibrils follow the Langmuir model (refer to Figure 2b), and the Langmuir isotherm has the following form is commonly used to describe adsorption data at equilibrium (Eqution 1).[S1]

$$q_e = \frac{q_{max} K_L C_e}{1 + K_L C_e} \quad (1)$$

In which q_e and q_{max} are the the adsorption capacity of adsorbent at equilibrium (milligrams per gram) and its maximum value, C_e is the equilibrium concentration of adsorbate in solution (moles per liter), whereas K_L is the Langmuir equilibrium constant of adsorption with units of liters per mole.

According to the fitted curve in Figure 2, the equation 1 could be expressed as

$$q_e = \frac{34.92 * 60.93 * C_e}{1 + 60.93 * C_e}$$

and thus, the q_{max} and K_L can be calculated and their values are 34.92 mg/g and 60.93 L/mol, respectively.

Additionally, according to the thermodynamic law, the Gibbs energy change (ΔG) of adsorption is calculated as follows

$$\Delta G = -RT \ln K_L \quad (2)$$

where T is the absolute temperature in Kelvin, and R is the gas constant with a value of 8.314 J · mol^{-1} ·K^{-1}. Therefore, the ΔG can be calculated and the value is approximately 10.21 kJ/mol, which is the interaction energy between IP6 and collagen fibrils.

References

[1] Liu, Y. Is the Free Energy Change of Adsorption Correctly Calculated? *J. Chem. Eng. Data* **2009**, *54* (7), 1981-1985.