Supporting Information

Simultaneous Hydrothermal Bioactivation with Nano-topographic Modulation of Porous Titanium Alloy towards Enhanced Osteogenic and Antimicrobial Responses

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Figure S1. SEM images of (a) STPP and (b) Ca(OH)₂ treated surface

Table S1. Surface elemental composition of modified Ti6Al4V by low resolution XPS

| Samples - | Elemental composition (% Atomic) | | | | | | | | |
|-----------|----------------------------------|------|------|-------|------|------|------|------|--|
| | Ti K | Al K | V K | O K | C K | Ca K | P K | Ca/P | |
| Т3 | 47.15 | 0.15 | 1.66 | 36.95 | 6.45 | 4.42 | 3.22 | 1.37 | |
| T4 | 63.2 | 0.49 | 2.27 | 24.7 | 4.21 | 3.04 | 2.09 | 1.45 | |
| T5 | 48.27 | 0.16 | 1.25 | 35.47 | 6.89 | 4.98 | 2.98 | 1.67 | |
| T6 | 41.3 | 0.34 | 1.33 | 41.7 | 7.23 | 5.95 | 2.15 | 2.77 | |



Figure S2. Layer thickness of nanostructures developed on treated (a) T3 (b) T4 (c) T5 and (d) T6 samples surface



Figure S3. (a) XPS profile and (b) XPS peak fitting of Ti 2p, O 1s, Ca 2p, P 2p for hydrothermally treated ($(STPP/Ca(OH)_2 \text{ at } 1/0.78 \text{ for } 120 \text{ min})$) porous Ti6Al4V samples



Figure S4. XRD analysis of (a) Ca(OH)2 (b) STPP (c) precipitates after mixing of STPP and Ca(OH)2 at 1:0.78 ratio (d) precipitates after hydrothermal treatment of STPP/Ca(OH)2 mixture (1:0.78)

| Samples | OSP | AFM | | | |
|-----------|---------------------|---------------------|--|--|--|
| | R _q (μm) | R _q (nm) | | | |
| UT | 1.61±0.31 | 41.3±2.7 | | | |
| Т3 | 2.91±0.55 | 101.0±8.4 | | | |
| T4 | 2.54±0.62 | 53.2±3.5 | | | |
| Т5 | 3.68±0.71 | 122.0±10.2 | | | |
| T6 | 5.31±0.83 | 129.0±13.6 | | | |

Table S2. Micro- and nano-roughness profiles of untreated and hydrothermally treated dense Ti6Al4V samples



Figure S5. Representative plots from adhesion studies of treated Ti6Al4V (T5) sample (a) Normal force vs. Time (b) Normal displacement vs. Time (c) Lateral force vs. Time (d) Lateral displacement vs. Time and (e) Friction coefficient vs. Time

| Samples | Interval | Layers | VV | MV | BV | TV | BV | VV | MV |
|---------|----------|--------|--------------------|--------------------|--------------------|--------------------|------|------|------|
| _ | | - | (mm ³) | (mm ³) | (mm ³) | (mm ³) | (%) | (%) | (%) |
| Control | 4 weeks | L 1 | 21.3 | - | 5.88 | 27.2 | 21.6 | - | - |
| | | L 2 | 22.7 | - | 4.71 | 27.4 | 17.2 | - | - |
| | | L 3 | 26.2 | - | 1.17 | 27.4 | 4.3 | - | - |
| | 12 weeks | L 1 | 9.98 | - | 3.23 | 13.2 | 24.5 | - | - |
| | | L 2 | 10.46 | - | 2.84 | 13.3 | 21.4 | - | - |
| | | L 3 | 11.55 | - | 1.69 | 13.2 | 12.8 | - | - |
| UTp | 4 weeks | L 1 | 1.79 | 0.52 | 1.33 | 3.64 | 36.5 | 49.2 | 14.3 |
| | | L 2 | 2.46 | 0.78 | 0.92 | 4.16 | 22.1 | 59.1 | 18.8 |
| | | L 3 | 1.59 | 0.49 | 0.55 | 2.63 | 20.9 | 60.5 | 18.6 |
| | 12 weeks | L 1 | 2.07 | 0.73 | 2.24 | 5.04 | 44.4 | 41.1 | 14.5 |
| | | L 2 | 1.58 | 0.49 | 1.07 | 3.14 | 34.1 | 50.3 | 15.6 |
| | | L 3 | 1.40 | 0.39 | 0.58 | 2.37 | 24.5 | 59.1 | 16.5 |
| Тр | 4 weeks | L 1 | 1.48 | 0.29 | 1.36 | 3.13 | 43.5 | 47.3 | 9.3 |
| | | L 2 | 1.45 | 0.30 | 0.87 | 2.62 | 33.2 | 55.3 | 11.5 |
| | | L 3 | 2.03 | 0.23 | 0.69 | 2.95 | 23.4 | 68.8 | 7.8 |
| | 12 weeks | L 1 | 0.84 | 0.36 | 1.25 | 2.45 | 51.0 | 34.3 | 14.7 |
| | | L 2 | 1.08 | 0.38 | 1.37 | 2.83 | 48.4 | 38.2 | 13.4 |
| | | L 3 | 1.80 | 0.36 | 1.17 | 3.33 | 35.1 | 54.1 | 10.8 |

Table S3. Assessment of quantitative bone ingrowth in different layers of bone defects at different time intervals

Void volume (VV), bone volume (BV), metal volume (MV) and total volume (TV)



Figure S6. Mechanism of tripolyphosphate (TPP) hydrolysis (scheme 1) and hydroxyapatite formation (scheme 2) during hydrothermal treatment of STPP and Ca(OH)₂ reaction mixture



Figure S7. EDX analysis of bare nanostructure and nano-deposit (T5)



Figure S8. (a) Hardness and modulus of treated surface by nanoindentation (b) contact angle of untreated and hydrothermally treated Ti6Al4V