#### **Electronic supplementary information**

### Appropriate regulation of magnesium on hydroxyapatite crystallization

# in simulated body fluids

Shuqin Jiang,<sup>a</sup> Yuanyuan Cao,<sup>a</sup> Chenxi Zong, <sup>b</sup> Yuanfeng Pang<sup>\*a</sup> and Zhiwen Sun<sup>\*a</sup>

<sup>a</sup> School of public health, and department of Toxicology, Capital Medical University, Beijing 100069, China

<sup>b</sup> School of Basic Medicine, Capital Medical University, Beijing 100069, China

\* Email: yuanfengpang@163.com ; zwsun@ccmu.edu.cn

#### **Tables**

Table S1. The composition of simulated body fluid (SBF).

Ion.	Na <sup>+</sup>	$\mathbf{K}^+$	$Mg^{2+}$	Cl-	<b>SO</b> <sub>4</sub> <sup>2-</sup>	Ca <sup>2+</sup>	HPO <sub>4</sub> <sup>2-</sup>	HEPES
C/mM	140	5.0	0-1.5	148-151	0.5	5.0	3.0	10.0

Table S2. The chemical analysis of Mg in ACP and HAP in the presence of different  $Mg^{2+}$  concentrations in SBF solution, or adding 0.5 mM  $Mg^{2+}$  at different reaction times.

Group	Mg/Ca molar ration in ACP	Mg/Ca molar ration in HAP	
	$(\text{mean} \pm \text{s.d.})$	$(\text{mean} \pm \text{s.d.})$	
0.2 mM Mg	0.019 + 0.004	$0.017 \pm 0.002$	
0.2			
0.5 mM Mg	$0.032 \pm 0.002$	$0.029 \pm 0.002$	
1.0 mM Mg	$0.058\pm0.005$	$0.040\pm0.005$	
1.5 mM Mg	$0.070\pm0.005$	$0.047\pm0.003$	
adding(0)	$0.032 \pm 0.002$	$0.029 \pm 0.002$	
adding(5)	$0.013\pm0.001$	$0.032\pm0.001$	
adding(10)	$0.010\pm0.001$	$0.028\pm0.001$	
adding(15)	$0.008\pm0.002$	$0.028\pm0.002$	

	20(002) (deg.)	(002) d-space (nm)	c lattice parameter (nm)	lattice distortion (%)
HAP (control)	25.889	0.3438	0.6875	control
$0.2~\mathrm{mM}~\mathrm{Mg}^{2+}$	25.911	0.3434	0.6869	-0.09
$0.5~\mathrm{mM~Mg^{2+}}$	25.924	0.3433	0.6866	-0.13
$1.0~\mathrm{mM~Mg^{2+}}$	25.938	0.3431	0.6863	-0.18
$1.5 \mathrm{~mM~Mg^{2+}}$	25.978	0.3425	0.6850	-0.36

Table S3. The (002) d-spacing, *c* lattice parameter, and lattice distortion of HAP and Mg-doped HAP. The shrinkage of the *c* lattice (lattice distortion) is calculated by [c(Mg) - c(control)] /  $c(control) \times 100\%$ .

## **Figures**



**Fig. S1** HAP crystallization process in the SBF solution with 0.5 mM Mg<sup>2+</sup>. (a) A typical pH curve; FTIR (b), XRD (c), and TEM (d-g) characterization of mineral formed in stage I,  $t_i$  (induction time), II, and III.



Fig. S2 FTIR (a) and XRD (b) characterization of final minerals formed at different  $Mg^{2+}$  concentrations.



Fig. S3 The pH curves of SBF solution by adding different Mg<sup>2+</sup> concentrations.



**Fig. S4** The morphology of ACP formed at different reaction times at induction period (in stage I) in control group. (a) 5 min; (b) 10 min; (c) 15 min.



Fig. S5 The pH curves of SBF solution by adding 0.5 mM Mg<sup>2+</sup> at different reaction times.



**Fig. S6** FTIR (a), XRD (b), and TEM (c-e) characterization of final minerals formed by adding  $Mg^{2+}$  after ACP formation at 5 min, 10 min and 15 min.



**Fig. S7** The enlarged view of (002) diffraction peak in XRD patterns (Fig. S2b<sup>+</sup>). The (002) diffraction angle is slightly increased with the increasing Mg<sup>2+</sup> concentration.



**Fig. S8** The enlarged view of (002) diffraction peak in XRD patterns (Fig. S2b<sup> $\dagger$ </sup> and Fig. S6b<sup> $\dagger$ </sup>). The (002) diffraction angle is not evident change when adding 0.5 mM Mg<sup>2+</sup> at different reaction times.



Fig. S9 The change of  $Mg^{2+}$  concent in ACP by adding 0.5 mM  $Mg^{2+}$  at different reaction times.



**Fig. S10** Scheme of the calculation of splitting function (SF).  $A_1$  is the area enclosed by the spectrum and the straight line and  $A_2$  is the area enclosed by spectrum and straight baseline, the SF is defined as the radio of  $A_1$  to  $A_2$ . SF is used as the crystallization indicator of calcium phosphate.