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## PAPER

## Synthesis and structure of iron- and strontium-substituted octacalcium phosphate: effects of ionic charge and radius

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## **Supplementary Information**



Fig.S1 XRD pattern of the product obtained at the reaction time of 10 min.

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Fig.S2 XPS survey spectra of undoped OCP, Fe-OCP and Sr-OCP.

Tab.S1 Elemental compositions of reactants and expected molar ratios for the synthesis of undoped OCP, Fe-OCP and Sr-OCP.

Samples	Ca (mM)	P (mM)	M (mM)	M/(M+Ca) molar ratio*	(M+Ca)/P molar ratio
undoped OCP	40	30	0	0	1.33
Fe-OCP	38	30	2	0.05	1.33
Sr-OCP	38	30	2	0.05	1.33

\* M stands for Fe or Sr.

Tab.S2 Diffraction angles and main characteristic peaks and corresponding crystal space of undoped OCP, Fe-OCP and Sr-OCP

Samples	Miller Index	Diffraction angle (°, 2ϑ)	FWHW (°, 2ϑ)	Interplanar spacing (Å, d <sub>hkl</sub> )
undoped OCP	(100)	4.7191	0.1786	18.7247
	(700)	33.5039	0.1624	2.6746
Fe-OCP	(100)	4.6437	0.1965	19.0285
	(700)	33.4400	0.1624	2.6796
Sr-OCP	(100)	4.6904	0.1625	18.8392
	(700)	33.4566	0.1299	2.6783

Tab.S3 Quantification analysis of compositions of surface of undoped OCP, Fe-OCP and Sr-OCP

Samples	Ca (mol.%)	P (mol.%)	M* (mol.%)	(Ca+M)/P molar ratio	M/(Ca+M) molar ratio (%)
undoped OCP	11.90	8.30	-	1.434	-
Fe-OCP	9.65	8.14	1.29	1.343	11.792
Sr-OCP	11.15	8.00	0.10	1.406	0.897

\* M stands for Fe or Sr.

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