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Metal-Doped β-Tricalcium Phosphate for Multifunctional Applications

Structural and Spectroscopic Insights

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Academic dissertation

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Abstract

Structure–property relationships are a fundamental concept in the design of novel materials for multifunctional applications. The ability to control and modify the properties of materials relies on the understanding of these relationships, given that a minor change in the material structure induces substantial differences in its properties. β-Tricalcium phosphate (β-TCP) is a promising multifunctional material with a flexible crystal structure comprising multiple Ca sites available for cationic substitution. This flexibility has sparked intensive research efforts to explore the possibilities of tuning its functional properties via metal doping. Despite these efforts, the structure–property relationships in metal-doped β-TCP remain not fully understood. This can be attributed to the complexity of the β-TCP crystal structure and to the limited data on the factors governing doping characteristics. Therefore, a systematic investigation is essential to accurately determine the effects of doping on the structure, properties, and potential of this versatile material.

This thesis establishes a comprehensive foundation for understanding the structure–property relationships of β-TCP and its metal-doped variants. Zinc (Zn) and copper (Cu) were chosen as dopants, and their effects on the structure and properties of the material were studied. A three-stage solid-state synthesis method for producing high-purity materials was developed using a combination of thermodynamic equilibrium calculations and experimental trials. The synthesized materials were extensively characterized using various analytical techniques for accurate determination of their properties. The structural investigations revealed that doping of Zn^{2+} and Cu^{2+} in β-TCP induced a shrinkage in its unit cell. These divalent metals were confirmed to occupy Ca4 and Ca5 in the unit cell, and their site occupancy preference was found to be concentration-dependent. The observed vibrational characteristics suggested a reduction in the symmetry of the P1 site due to the substitution of calcium (Ca) ions by the dopants at the neighbouring Ca4 site. The morphology of the materials exhibited minor changes characterized by non-uniform grain size. The optical investigations revealed that the host matrix effect dominated the optical absorption characteristics of the doped materials with a slight reduction in the band gap energy. On the other hand, the photoluminescence properties of β-TCP were significantly altered by the metal doping. Cu-doped variants exhibited well-defined emissions in the visible range. In contrast, low-intensity emissions were detected for Zn-doped samples. The photocatalytic activity of β-TCP and its Zn-doped counterparts was investigated for the degradation of organic dyes. The Zn-doped materials demonstrated clear improvement in the photocatalytic performance as compared to the host material. Finally, the frequency-dependent electrical characteristics of the materials were investigated in detail. The results showed that doping of Zn^{2+} and Cu^{2+} notably enhanced the charge storage and conduction capability of β-TCP. The materials displayed a non-Debye relaxation that was attributed to grain and grain boundary contributions.

This thesis demonstrates the potential of metal-doped β-TCP as a multifunctional material and can guide future efforts to meet the emerging demands of sustainable materials design and applications.

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β-tricalcium phosphate, zinc, copper, doping, thermodynamic equilibrium calculations, crystal structure, photoluminescence, photocatalysis, impedance spectroscopy.

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