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DFT, MP2 and MP4 Investigations of Calcium Phosphates (X3(PO4)2, X=Ca, Mg, Zn, Sr) Materials for Biomedical Applications

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Abstract

β-Tricalcium Phosphate [β-TCP), Ca3(PO4)2] material has gained much interest in recent clinical applications, as they are mainly used to repair and replace the injured part(s) of human teeth and bones. However, Ca3(PO4)2 compound shows less stability, brittleness and bioactivity to stimulate natural bone growth in an acceptable manner; thus their clinical performance is reduced. Therefore, in the present study, we have replaced Ca element of Ca3(PO4)2 compound with Mg, Zn and Sr elements to obtain Mg3(PO4)2 (Magnesium Phosphate), Zn3(PO4)2 (Zinc Phosphate) and Sr3(PO4)2 (Strontium Phosphate), to use in bone and dental applications referring to their similar chemical composition to the natural bones and teeth. To achieve this, the electronic, cohesive energy, geometry optimization, thermodynamic and optical properties of X3(PO4)2 (X = Ca, Mg, Zn, Sr) compounds are theoretically investigated using full-potential linearized augmented plane wave method (FP-LAPW) within the generalized gradient approximations (GGA) under DFT framework. Additionally, HF, MP2, MP4, TD-DFT and several DFT calculations are performed along with different basis set. The calculations of basis set superposition error (BSSE) are performed to get more accurate cohesive energy values of the considered materials. The cohesive energy calculations reveal that X3(PO4)2 (X= Mg, Zn, Sr) compounds are more stable based on their larger negative cohesive energy values compared to Ca3(PO4)2 compound. The obtained results are quite promising for increasing the quality of these materials and provide more evidence to synthesize/fabricate novel biomaterials for medical and dental applications.

Biography:

Adam Mohammed Adam Bakheet has expertise in the theoretical and computational Materials Science field including: (a)Theoretical design of biomaterial devices with novel functions for dentistry and medicine applications, (b) Design and investigation of fundamental properties of materials exploited in medical applications. (c) Performing several ab-initio calculations to investigate the fundamental physical and chemical properties of Calcium Phosphate materials at the ground and excited states. (d) Doping the pure Calcium Phosphate materials with some trace elements such as Zinc, Magnesium, Strontium, and Silicon.

Speaker Publications:

1. A. M. A. Bakheet, L. Mohammed, M. A. Saeed, A. Musa, H.A. Rahnamaye Aliabad (2018), Ab-initio Study of Chemical and Physical Properties of Pure, Sr, and Zn-Doped β-Tricalcium Phosphates for Biomedical application. ISSN (Print): 2476-8316, ISSN (Online): 2635-3490.
2. Adam Mohammed Adam Bakheet, Mohammad Alam Saeed, Isa, Ahmad Radzi Bin Ma Isa and Riadh Sahnoun (2016), First-principles study of the physical properties of pure and doped calcium phosphate biomaterial for tissue engineering. doi:http://dx.doi.org/10.1016/B978-0-323-42862-0.00007-9.
3. A. M. A. Bakheet, M. A. Saeed, Riadh Sahnoun, A. R. M. Isa, Lawal Mohammed, and Tariq Mahmood, (2015), "Density Functional Theory Study of the Electronic and Optical Properties of Pure and Magnesium Doped β-Tricalcium Phosphate Compound. ISSN:2180-3722
4. A. M. A. Bakheet, M. A. Saeed, A. R. M. Isa, R. Sahnoun, "Theoretical Investigations of β-Tricalcium Phosphate Biomaterials". Jurnal Teknologi Vol. 78, No. 3-2, (2015), ISSN:2180-3722. Status: Published, doi: http://dx.doi.org/10.11113/jt.v78.7836.

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