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Computational modeling and studies of hydroxyapatite with defects of the oxygen vacancy type providing its photocatalytic activity

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A new model of the structure of hydroxyapatite (HAP) with defects of the oxygen vacancy type and hydroxyl group vacancy type has been developed. The model made it possible to explain the change in the optical properties of the HAP and provide for the mechanism of its photocatalytic activity. The obtained new results and knowledge allow us to already purposefully change the optical properties of HAP (introduction of the necessary type of the defects) and control the photocatalytic activity of HAP, which is extremely important for many practical applications (in the cleaning the environment, including the water from harmful impurities and components, in the chemical photocatalytic synthesis, in the antimicrobial treatment, etc.). The model is developed on the basis of several new approaches to the density functional theory (DFT) with combined application of the various hybrid and exchange-correlation functionals, and also taking into account the Coulomb shielding of the defect charge, which allows made more exact and accurate calculation of structural, optical and other properties of HAP materials. These approaches continue to develop on some new more complex models of the super-cells of HAP, which will allow us to obtain a number of even more highly accurate results of calculations of the HAP properties for both pure and with different defects. The computed properties of HAP material with super-cell model (2x2x2 - 8 unit cell) are considered using semi-local (PBE potential) and hybrid exchange-correlation functionals with different fraction of exact exchange contribution. The excitation properties are compared with the results of GW-approximation method for calculation of quasi-particle band structure. It was shown that optical properties of bulk HAP are best described using B3LYP exchange-correlation functional and for pure HAP have band gap Eg ~ 7.3 eV, while with O vacancy it is lowered.

Recent Publications:

1. Bystrov V S, Coutinho J, Bystrova A V, Dekhtyar Y D, Pullar R C, Poronin A, Palcevskis E, Dindune A, Alkan B, Durucan C and Paramonova E V (2015) Computational study of hydroxyapatite structures, properties and defects. J. Phys. D: Appl. Phys. 48:195302.
2. Bystrova A V, Dekhtyar Yu D, Popov A I, Coutinho J and Bystrov V S (2015) Modified hydroxyapatite structure and properties: modeling and synchrotron data analysis of modified hydroxyapatite structure. Ferroelectrics 475(1):135-147.
3. V S Bystrov, C Piccirillo, D M Tobaldi, P M L Castro, J Coutinho, S Kopyl and R C Pullar (2016) Oxygen vacancies, the optical band gap (Eg) and photocatalysis of hydroxyapatite: comparing modelling with measured data. Applied Catalysis B: Environmental. V 196:100–107.
4. V Bystrov, A Bystrova and Yu Dekhtyar (2017) HAP nanoparticle and substrate surface electrical potential towards bone cells adhesion: Recent results review. Advances in Colloid and Interface Science 249:213-219.
5. V S Bystrov et al. (2017) Surface modified hydroxyapatites with various functionalized nanostructures: computational studies of the vacancies in HAP. Ferroelectrics 509:105–112.

Biography

Vladimir S Bystrov has completed PhD, Dr. Habil.Phys. Dr.Sci. Phys. & Math. from Russian Academy of Sciences. Since 1993, he has his expertise in various fields of computational molecular modeling, computational exploration and computer simulation of nonlinear multifunctional nanomaterials and different organic & bio-molecular nano-structures such as: bioferroelectric & polymer PVDF/PVDF-TrFE thin ferroelectric films, graphene/oxide graphene and related polar composite nanomaterials; amino acids (glycine, etc.), peptides nanotubes, thymine & DNA; hydroxyapatite (HAP) & nanoparticles, etc. Computational studies of nanostructures were made using the molecular mechanics, quantum-chemical calculations (ab initio, DFT, semi-empirical methods), molecular dynamics (MD) on the base of various software (HyperChem, AIMPRO, VASP, etc.) and clusters in Russia IMPB & KIAM, Linux cluster in University of Aveiro, Portugal. He is a Head of the Group for Computer Modelling of Nanostructures and Biosystems of IMPB-KIAM RAS, Pushchino.

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