Can Quantum-Mechanical Calculations Shed Light on Biomaterials?

Hydroxyapatite, bioglasses and functionalized silica surfaces interacting with biomolecules

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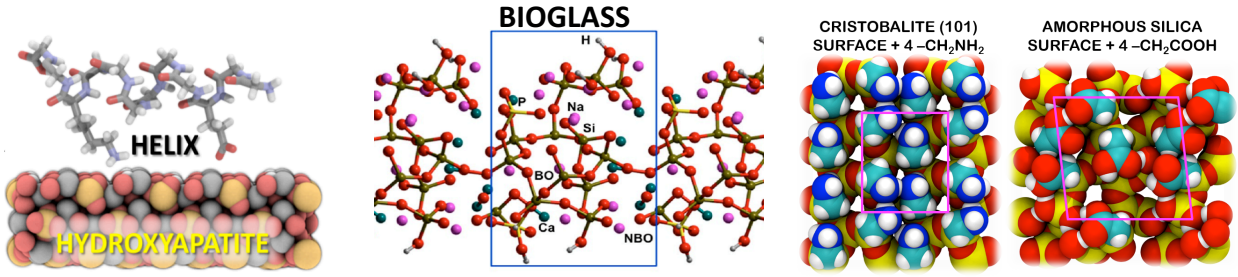
The increasing life expectancy, the growing senior population and more generalized wealth are only some of the many driving forces for the current strong effort in the research area of biomaterials. Indeed, improved biocompatible, bioactive, antimicotic, antiseptic and antibacterial materials are needed for substituting aged or injured tissues of the human body, as well as for the cure of diseases affecting them. In this context, theoretical methods can be successfully applied to provide structural information and surface properties at an atomistic level and be compared with experimental measurements.

In the present contribution, recent applications of periodic DFT simulations will be shown, ranging from various surfaces of hydroxyapatite - the main constituent of the inorganic phase of bones and teeth - in interaction with several biomolecules, to the investigation of bioglasses of different chemical compositions, both bulk and surfaces, relevant as inorganic materials in the prosthetic field. The cases of acidic, basic and quinone-based functionalized silica surface models for subsequent condensation of organic molecules or amino acids, to be applied as anti-bacterial coatings for dental implants, will complete this broad and challenging scenario.

The structure of active sites, the H- bonding pattern, the relative stability and the interaction energy, as well as the electronic properties are some of the results that can be derived by our quantum-mechanical calculations. Moreover, the simulation of IR spectra of the various models provides a direct comparison with the experimental data measured on the real samples, helping in the interpretation of the reaction mechanisms occurred at the different surfaces or interfaces.



The joint use of experimental and computational techniques has indeed revealed very effective to improve in the field of biomaterial interfaces, specifically in the understanding of biological complex systems and mechanisms.

References

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