Abstract

iMedPub Journals
www.imedpub.com

Nano Research & Applications
ISSN 2471-9838

2021
Vol.7 No.S3

From biomaterial interfaces to hydrogen storage hydrides: How quantum-mechanical calculations can shed light on advanced materials

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Abstract

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. Another current and dramatic challenge is the development of good, clean, and efficient materials for energy storage, decreasing CO_2 emissions by using only renewable energies, instead of fossil fuels. Hydrogen-based solutions are promising key technologies to boost this energy transition, thereby improving energy storage efficiency. Recent evolutions in High Performance Computing (HPC) architectures and the concurrent development of more efficient quantum-mechanical softwares have dramatically increased the size and complexity of the systems that can be modeled by a variety of *ab initio* methods, at a very high accuracy level. One of the areas that greatly benefits from these advancements is materials science: surfaces and interfacial phenomena, defective solids, functional materials, and nano-particulate systems, all require models that are hardly handled by desktop computing architectures due to the large system size.

Some recent applications of periodic large-scale DFT simulations are presented, ranging from various the inorganic phase of bones and teeth - in interaction with several biomolecules, to the investigation of cyclodextrin-based nanosponges as drug carriers. The case of materials for solid-state hydrogen storage in alloys and inorganic materials 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 thermodynamic propertiesare can be derived by quantum-mechanical calculations.

Biography:

Experienced tenure-track PhD researcher with fifteen-year history of working in the higher education field (Academia). Skilled in computational chemistry, nanomaterial's, Research and Development (R&D), teaching, scientific and creative writing, with a Master focused in scientific communication and a great propensity to solve problems. Open to new collaborations.

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