Abstract

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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.

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 surfaces of hydroxyapatite - the main constituent of 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.

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*

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Biography

The Corno Marta is a BsC (Chemistry): Diploma di Laurea Triennale in Chimica – physical chemistry, Summa cum laude (110/110),with a thesis entitled “The tunnel effect in chemistry - L’effetto tunnel in chimica”, Università degli Studi di Torino. MsC (Chemistry): Diploma di Laurea Specialistica in Metodologie Chimiche Avanzate – molecular modelling,Summa cum laude (110/110), with a research thesis entitled “Ab-initio study of materials relevant for the Constitution of bioglasses - Studio ab initio di materiali rilevanti per la costituzione di biovetri”, Università degli Studi di Torino

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