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PhD Defense

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Towards the *Ab Initio* Simulation of Tendon and Bone Materials

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Abstract

Collagen protein is the most abundant protein in all vertebrate as it is found in plenty of different tissues with several functions. It aggregates as collagen fibril, which is the basic building block of the tendons and bones. The tremendous complexity of these natural composite materials hides extraordinary features in terms of mechanical properties. Clearly, understanding the nanoscale interface of bone and tendons at atomistic level can dramatically improve the development of bio-composites and our understanding of related diseases. Molecular dynamics technique based on classical force fields is the method of choice to study such a complex system, because it allows treating model system size approaching that of the real material. Nonetheless, the classical force fields are somehow of unpredictable quality, particularly for treating the interface layer between the inorganic and the organic components of this hybrid materials. At variance with the classical approach, we aim at elucidating the atomic features of bone and tendon main components, e.g. collagen, hydroxyapatite and water, by means of accurate simulations based on quantum mechanical methods (QM). This represents a challenging task due to the extreme complexity of the systems of interest and the well-known model size limits of QM. In this seminar, several strategies for using QM method in bone and tendon simulations are presented: from the test of a new promising “fast and accurate” QM approach, to fully exploit the helix symmetry of collagen protein models saving significant amount of computational resources. The long-term outcomes of this research work will provide to the scientific community robust atomistic models, structural and energetic data at an unprecedented level of accuracy. Our QM results allow to improve existing force fields based on classical mechanics, extending the accuracy of our results to system size close to the real composite systems.

Prof. Piero Ugliengo

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