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Seminar

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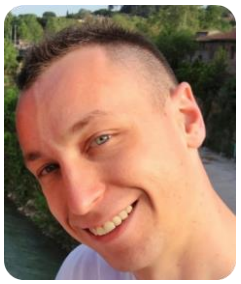

Closing the gap: enhanced sampling methods for the simulation of silica interactions with biomolecules

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Abstract

The interaction between biomolecules and inorganic materials has become of eminent interest in fields ranging from basic research up to industrial product design, leaving several open challenges. Proteins are known to undergo changes in their conformations upon interaction with solid material surfaces, with important effects on their activity. How these changes can be predicted and correlated to the physico-chemical feature of the material is however still unclear. Among inorganic materials, the interaction of silica with biological systems is particularly complex and contradictory. Indeed, on the one hand, silica is at the basis of several biomineralization processes, on the other hand, the contact of some types of silica with the membrane of erythrocytes is known to cause its rupture.

Molecular dynamics (MD) simulations are a valuable tool in investigating these aspects as well as other issues regarding the interaction of inorganic materials with biomolecules. However, despite the increase in available computational resources, MD still suffers a debilitating timescale problem that greatly reduces the number of phenomena that can be investigated. Numerous enhanced sampling methods have been introduced to alleviate this problem, such as Metadynamics (MetaD), Replica Exchange with Solute Tempering (REST) and Umbrella Sampling.

These methods will be briefly described in this seminar, and some examples of their applications will be presented, to shed light on the interactions between biomolecules, such as proteins and cell membranes, with silica, both as a solid surface and in nanoparticle form.

Prof. Piero Ugliengo

Prof. Marco Vincenti (Direttore Dipartimento di Chimica)