Water infrared spectrum at the interface with silicon and hydrogen-terminated silicon surfaces using molecular dynamics approach

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The interface between water and solid surfaces is of interest in biological systems and materials science [1-3]. In this interface, we can find a rich environment for the investigation of confinement of water molecules' motion, manifesting varying transport and vibrational properties as a result. The project Biowater has been focused on the development of new methods to characterise the interaction of biomaterials and water. Biowater has been concentrated on different classes of biomaterials and chemical imaging modalities, such as near infrared (NIR), mid-infrared (MIR) and Raman. Also, theoretical approaches have been used to provide information at the atomic level on structures that water adopts in the interface.

Understanding the water-biomaterial interaction, which occurs in the interface, provides us information related to hydrogen bonding, which is crucial to comprehend wetting phenomena [4]. However, the way in which the water builds the hydrogen-bonded network in this interface remains in controversy due to water's ability to establish numerous hydrogen bonds [5]. An approximation using a combination of experimental and theoretical methods may be useful to unravel the interface's interactions. On the one hand, Infrared (IR) vibrational spectroscopy allows understanding the hydrogen network in water ensembles [6]. On the other, when we use a full atom description in the force field, Classical Molecular Dynamics simulations (MDS) gives information related to the dynamical hydrogen bonding formation along time, and providing atomistic information related to the water biomaterial interaction.

In this work, MDS were performed to characterise bulk water (liquid, super-cooled and ice) and silicon-based materials in contact with water using the software package DL-POLY Classic for all simulations. The SPC/Fw model for water and Tersoff potential to describe the different silicon materials was used. Periodic boundary conditions in all three directions were imposed, while the van der Waals interaction (sphere of radius of 7.0 Å) and the standard energy and pressure long-range corrections were applied. For electrostatic interactions, the Ewald summation technique was adopted. The velocity Verlet algorithm was used to propagate the trajectory under constant temperature (220 and 300 K for bulk water and 300 K for water-silicon systems) and volume conditions (NVT ensemble) employing the Evans thermostat. Fourier transformation was applied to calculate the auto-velocity correlation function, which allows the power spectra to be obtained. IR spectra for all systems were obtained via the dipole autocorrelation function [7] and/or electrical flux approach [8]. We analyse these spectra, power and IR, to obtain information to make a correlation between the bulk water and water in contact with different silicon-based materials. A strong similarity between ice water and first water monolayer in contact with silicon power spectra has been found, suggesting that similar structures are adopted in both cases.

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