73rd MSS-Seminar

Wednesday, July. 1st, 15:30

Nägelsbachstr. 49b

MSS

Solvation-induced interactions at biological interfaces

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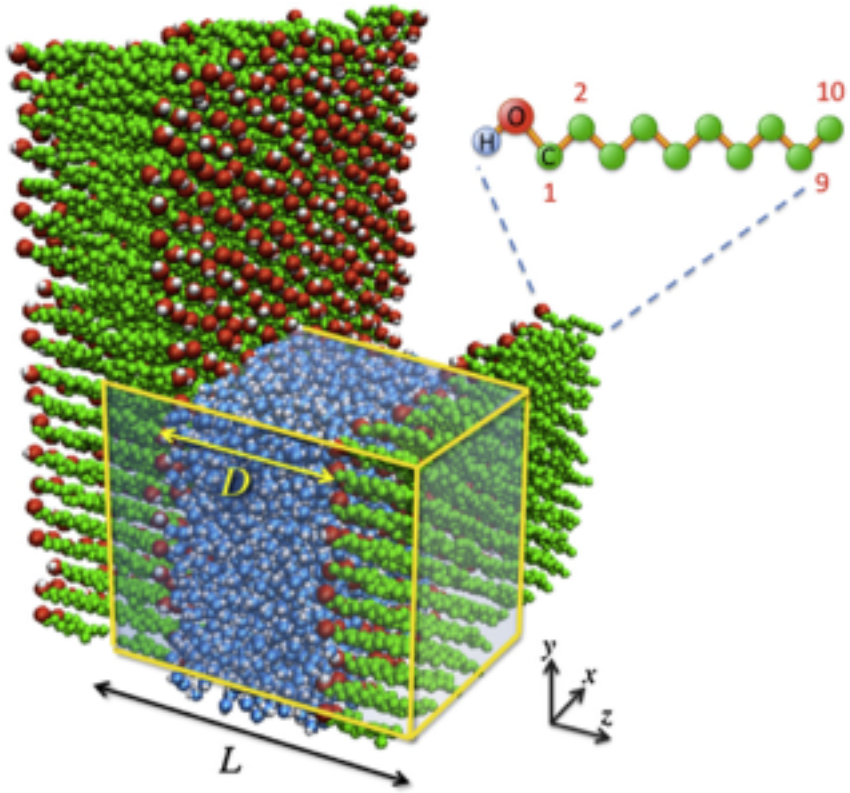

The molecular layer of water molecules on surfaces, the so-called hydration layer, is important for the properties of biological and technological surfaces. We study the interaction between two hydrated surfaces using a novel simulation technique that allows to efficiently determine the interaction pressure at prescribed water chemical potential. Prior research concentrated on the two limiting scenarios, namely hydrophobic attraction (or cavitation) between hydrophobic surfaces, and hydration repulsion for very polar (i.e. very hydrophilic) surfaces. Recent experiments demonstrated weak attraction between mildly hydrophilic surfaces, i.e. surfaces for which the contact angle is slightly smaller than 90 degrees, a finding that does not fit into the existing theoretical framework. Indeed, using atomistic simulations, we show that between the limiting regimes representing hydrophobic attraction and hydration repulsion an intermediate novel regime corresponding to hydrophilic attraction exists. Hydrophilic attraction occurs quite generally for surfaces that favorably interact with water and among themselves. Analysis of the hydrogen-bonding statistics shows that the balance between hydration repulsion and hydrophilic attraction is dominated by surface-water hydrogen bonds. For the important case of two dissimilar surfaces we constitute a universal phase diagram in terms of the surface contact angles, distinguishing the attractive and repulsive cases.