



Elitenetzwerk
Bayern



What do molecular simulations teach us about solvation forces?

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Solvation forces are important effects that determine, amongst many other phenomena, the self-assembly of proteins and other biological systems. In my talk I will discuss recent advances in the theoretical understanding of solvation forces in aqueous systems based on molecular simulations. I'll present an overview of the properties of water interfaces, the behavior of ions in bulk and at interfaces, and the salt influence on colloidal stability. In the last part, I present a simulation study of peptide desorption from surfaces by means of AFM single-molecule experiments.

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