Insights into the Molecular Composition of Ethanol-Water Liquid Mixtures through Electron Spectroscopy

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In this talk we present cylindrical micro-jet photoelectron spectroscopy (cMJ-PES) and theoretical simulations to study the properties of ethanol-water solutions at all concentrations [1], from 0 to 100 MOL% ethanol. Our goal was to better understand the microscopic structure and intermolecular bonding patterns of these mixtures. While ethanol-water solutions are widely used and studied, there is still controversy over the nature of their hydrogen bonding networks. We found that at low concentrations, ethanol molecules form a film on the surface, making it energetically favorable [2]. In bulk, up to 10M%, ethanol, oxygen atoms tend to form a third acceptor hydrogen bond to water molecules. At 20 M%, we have results pointing out for clathrate structures presence. At the surface, ethanol forms a closely packed layer between 5-25 M%. Above 85 M%, we have evidences that water tends to move to the surface, which explains the azeotrope effect [3]. We compared our findings with predictions from other spectroscopic techniques and highlighted the importance of an integrated approach combining molecular dynamics with quantum predictions for cMJ-PES measurements [4]. Our protocol can be applied to the study of other alcohol mixtures and binary solutions.

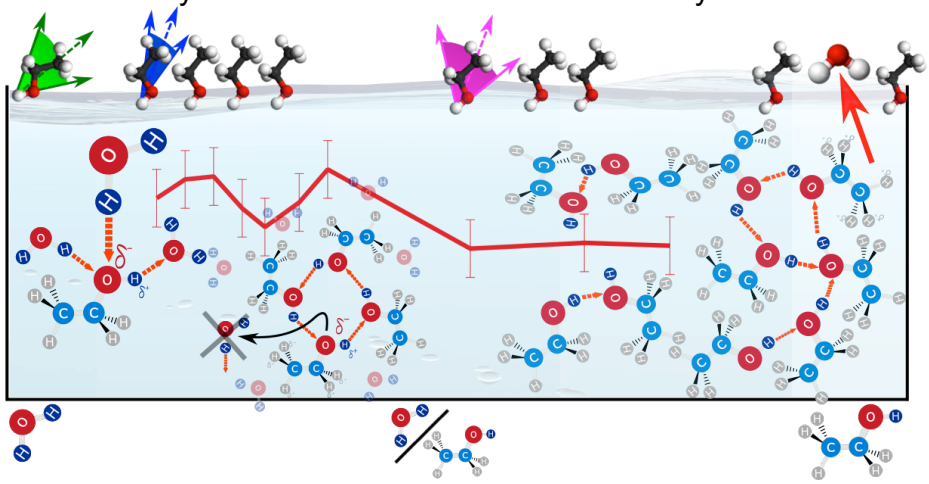

Figure 1: Ethanol-water mixtures, bulk and surface constitution reveled by a combination of experimental and theoretical calculation

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