Maximizing water-water interactions at aqueous interfaces: the 2D-HBond-Network

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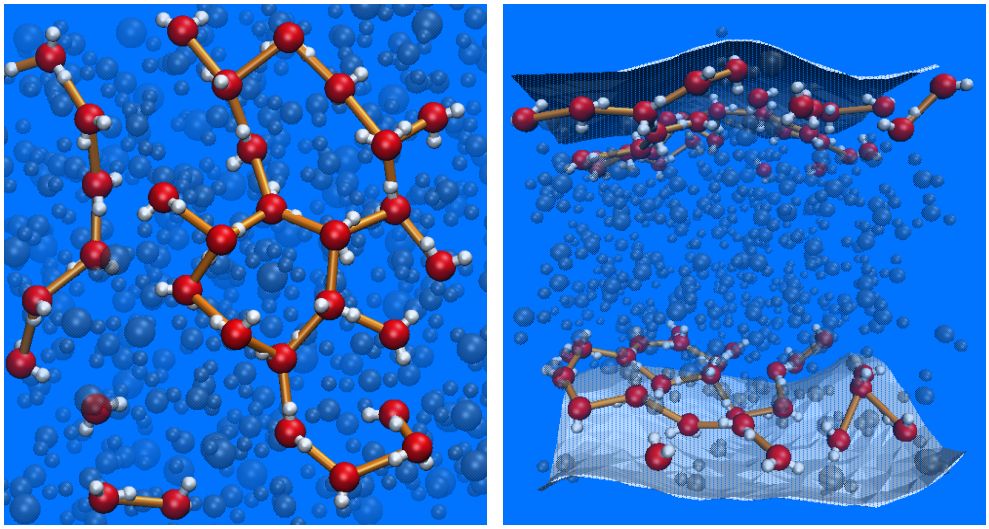
In the present lecture, a full rationalization of the arrangement of water (at the molecular level) at the interface with air is provided, by coupling Density Functional Theory (DFT) based Molecular Dynamics simulations (run with the CP2K package), Force Field based Molecular Dynamics Simulations (rigid SPC/E and flexible SPC/Fw models, Gromacs package) and vibrational Sum Frequency Generation Spectroscopy (vSFG).

In our recent works[1] we have revealed a specific H-Bond structure organization of the water molecules at the air/water interface: an extended 2-Dimensional H-Bond network (2DN), connecting all the water molecules in the topmost interfacial layer (roughly 3.5 A thickness) within an H-Bond structure parallel to the water surface. See the picture below[1]. The 2DN structure provides new elements to rationalize several properties specifically observed at the air/water interface: structural properties (water density, orientation), dynamical properties (specific H-Bond and orientational dynamics at the interface), physical properties (surface potential, surface tension, vSFG interfacial spectroscopic response) and chemical properties (charge separation and recombination, proton trapping and proton hopping).



[1] S. Pezzotti, D.R. Galimberti, M.-P.Gaigeot, J. Phys. Chem. Lett. 2017, 8, 3133–3141 ;
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