The ordering of water around hydrophobic solutes in electric fields

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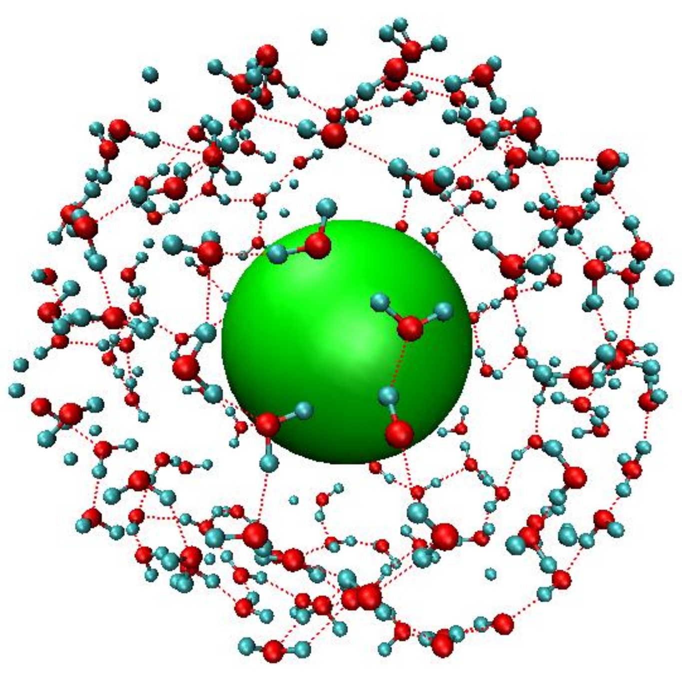
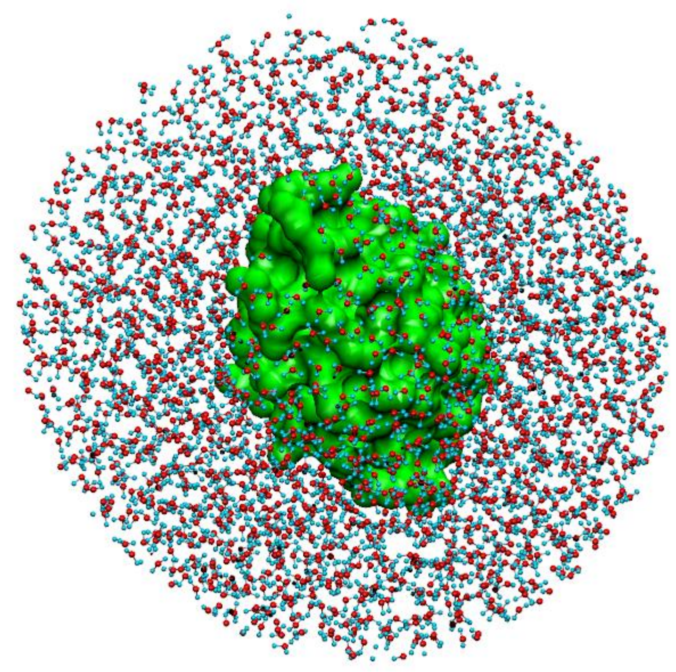
Introduction



Lennard-Jones particle first hydration shell

The understanding of nanoscale electrowetting is intimately related to the structure of water near a hydrophobic interface, which is also a key aspect of the hydrophobic effect [1]. Our goal is to investigate the effect of the electric field in solvation of the Lennard-Jones (LJ) particle in pure water and to compare the results with those of heptane droplets. All simulations were performed with GROMACS MD simulation package [2].



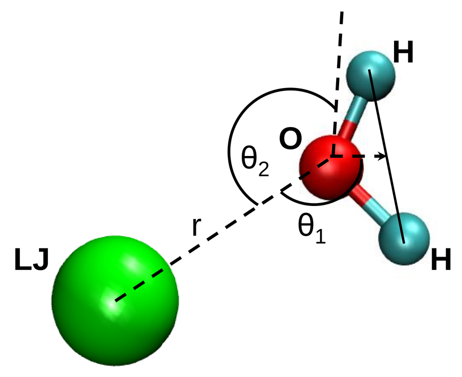
Heptane droplet in water

Packing of water around a particle

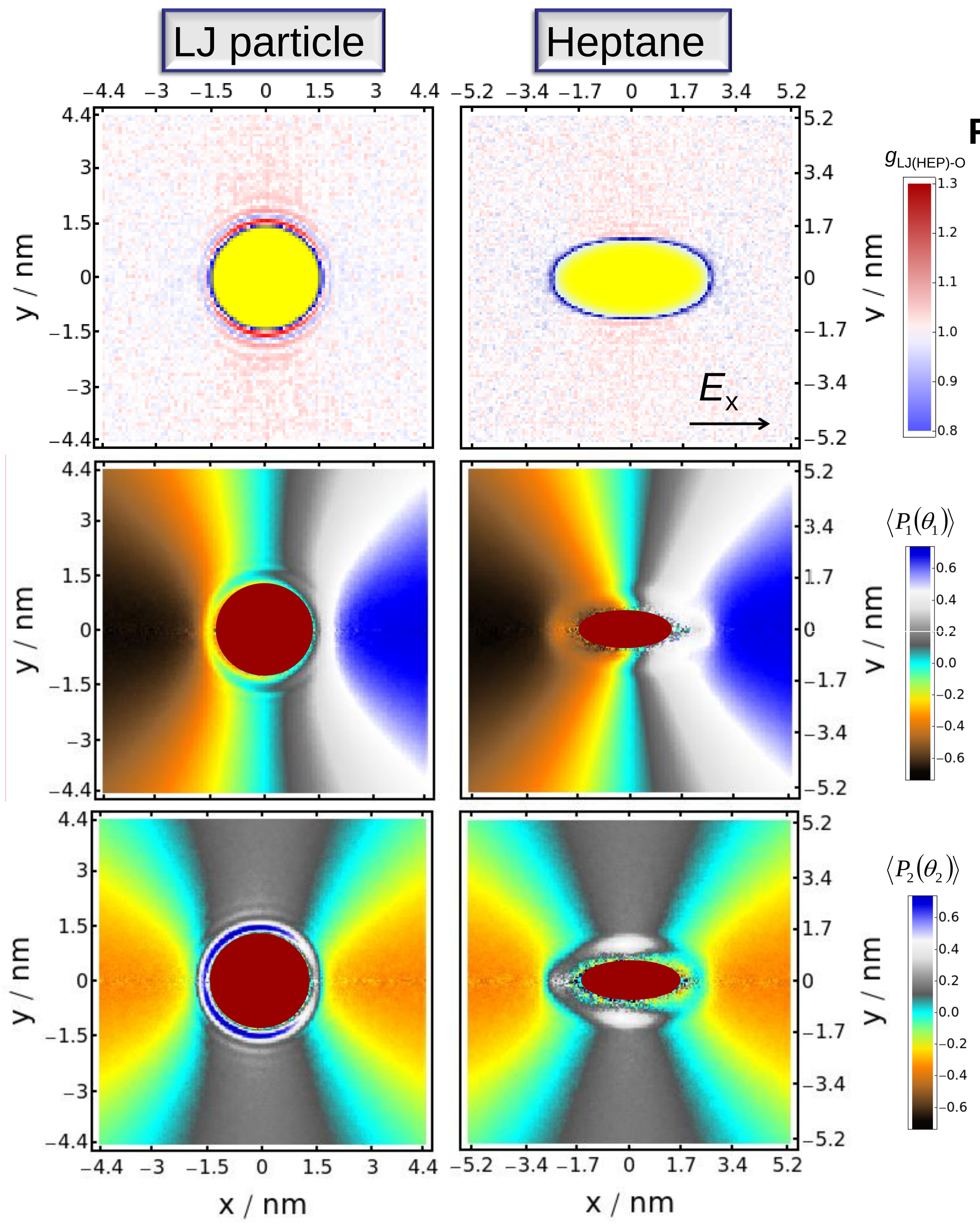
Correlation functions

$$P_{TOT}(r,\theta_1,\theta_2) = g(r,\langle P_1(\cos\theta_1)\rangle,\langle P_2(\cos\theta_2)\rangle)$$

give the probability for a water molecule to be in a specific orientation at a distance r from the center of mass of the particle [3].



The coordinate system



Radial distribution function

Ellipsoidal deformation

$r \in [0,\infty]$

$g(r+\Delta r)$

Dipole angle correlation function

$\theta_1 \in [0^\circ,180^\circ]$

$\langle P_1(r+\Delta r)\rangle = \langle \cos\theta_1 \rangle_r$

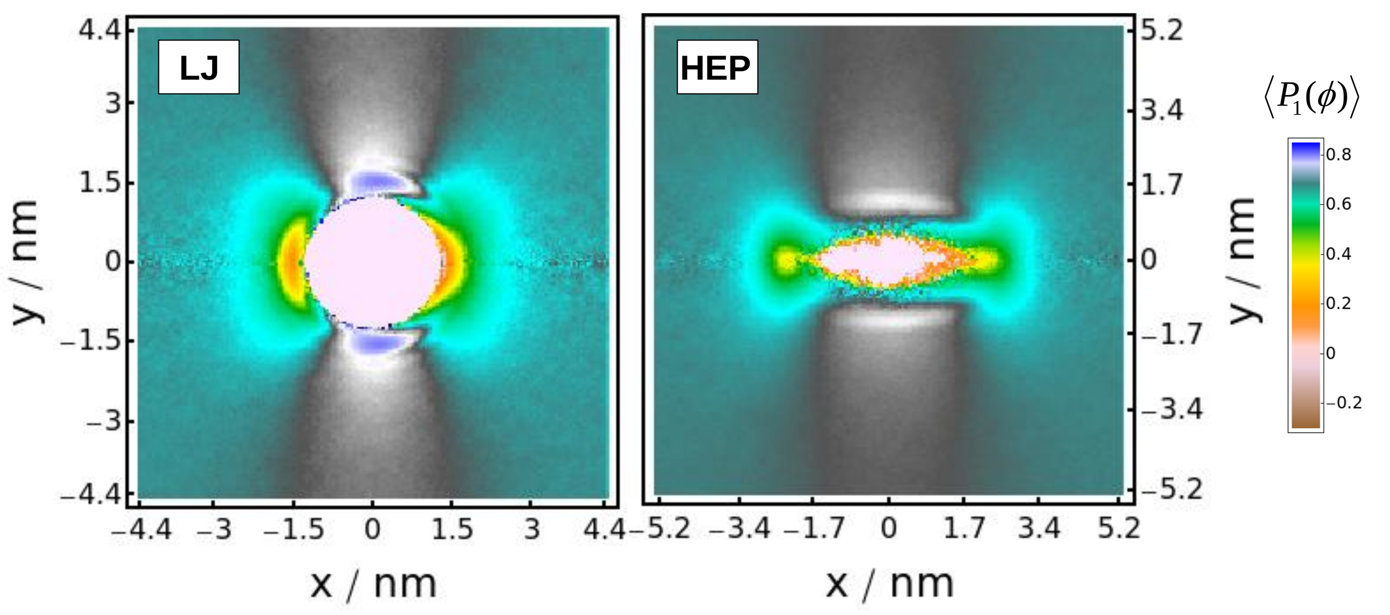
Normal angle correlation function

$\theta_2 \in [0^\circ,90^\circ]$

$\langle P_2(r+\Delta r)\rangle = \langle 3\cos^2\theta_2 - 1\rangle_r$

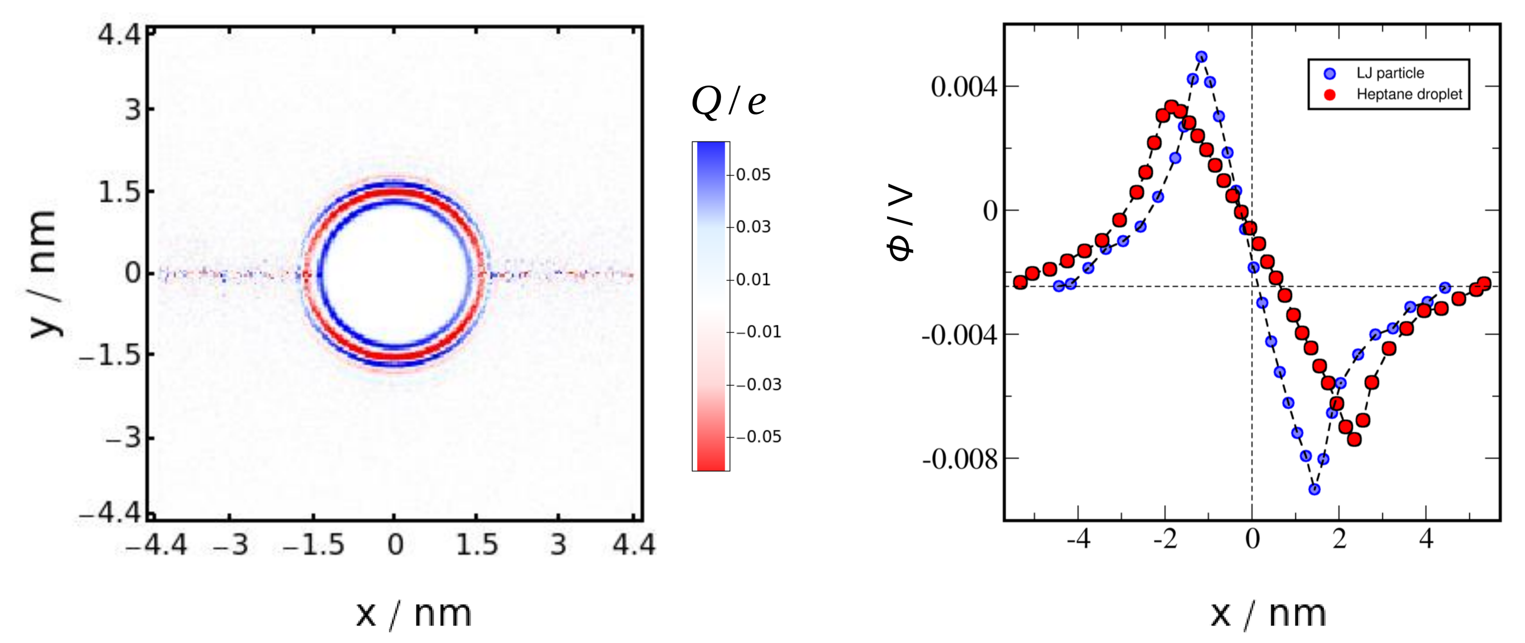
Charge and dipole density profiles

Mean projection of the water dipole vector onto the electric field vector



Pronounced –x/+x asymmetry

Charge density Q of the LJ particle (left) and electrostatic potential (right) along the line y=0 for the LJ particle and heptane droplet



Orientation of water with respect to the field competes with the orientation with respect to the solute particle and results in a complex pattern and low-density regions around at the +x and –x poles and a static electrostatic potential across the particle.

Conclusions

Water wets the hydrophobic surface more effectively when the applied field is parallel to the interface as compared to when the field is perpendicular to the interface, a result which is an agreement with previous findings in the study of water orientation between two hydrophobic walls [4]. The observed long-ranged field-induced correlations imply that for sufficiently high volume fractions, two hydrophobic particles in an electric field may sense and interact with one another by means of the ordered network of water molecules between them.

References

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