Electrophoretic mobility of hydrophobic particles

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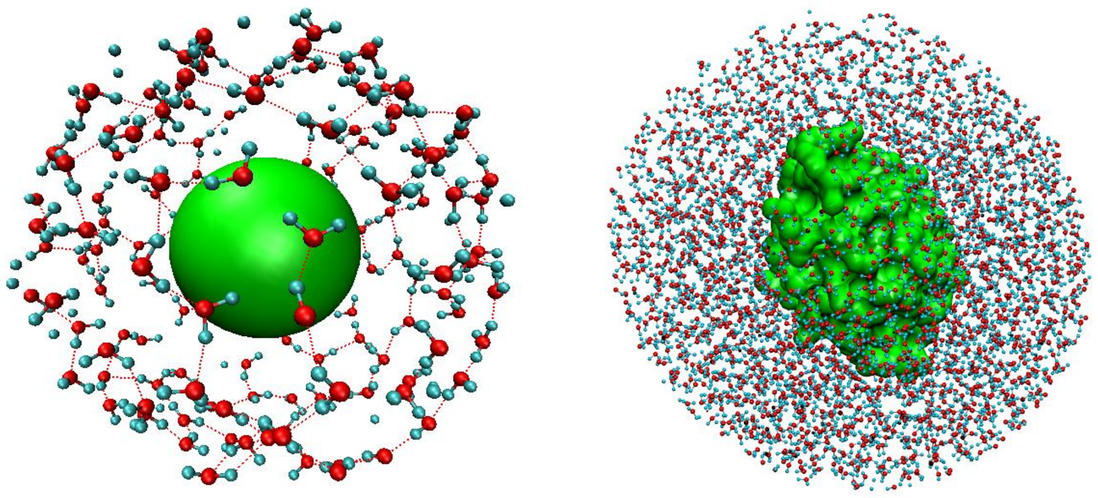
Introduction

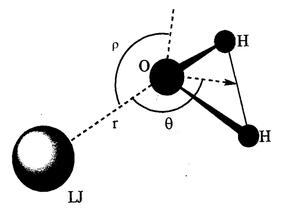
Hydrophobic objects, as oil droplets, show negative electrophoretic mobilities [1], the origin of which is not yet understood. Our goal is to investigate this effect for a Lennard-Jones particle (LJ) in pure water (no added ions) and to correlate the results with the mobility of heptane droplets [2]. All simulations were performed with GROMACS MD simulation package [3].



Water - Lennard-Jones particle first hydration shell (left), and a snapshot of a heptane droplet in water (right).

Long range effective interactions

Correlation functions are related to the probability of finding water molecules in a specific angular orientation at a distance **r** from the Lennard-Jones particle [4].



LJ-water coordinate system

Radial distribution function

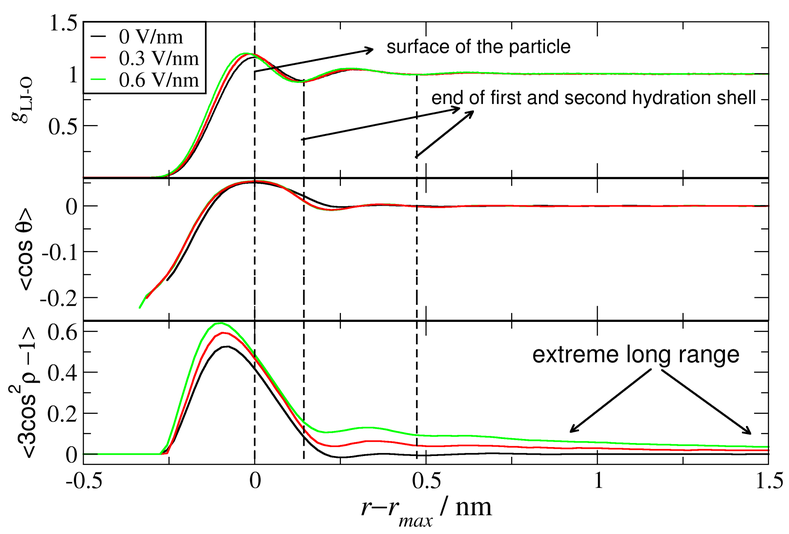
$$r \in [0, \infty]$$

Dipole angle correlation function

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

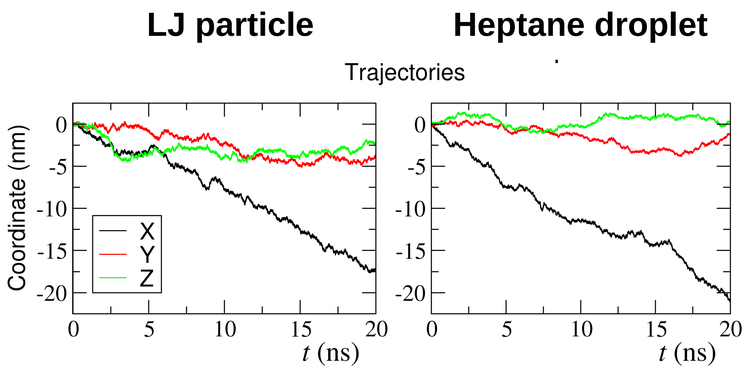
Normal angle correlation function

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

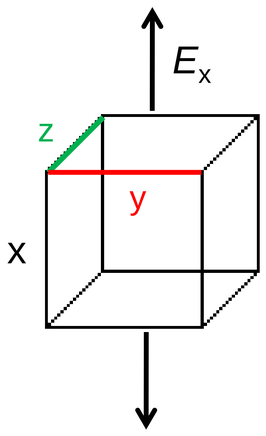


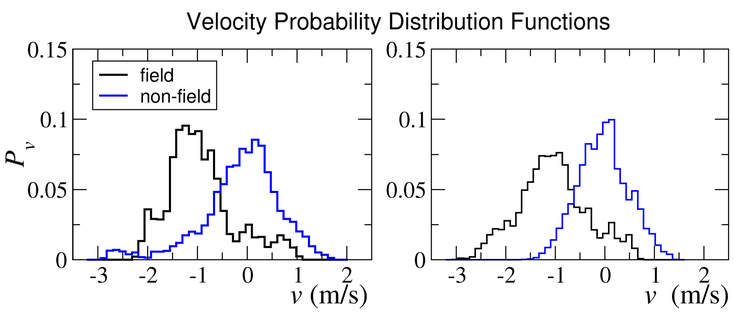
Extremely long-range correlations are induced by the electric field.

Migration of the particles in an electric field



Time displacements from *t* = 0 of LJ particle and a heptane droplet (radius *r* = 1.5 nm).

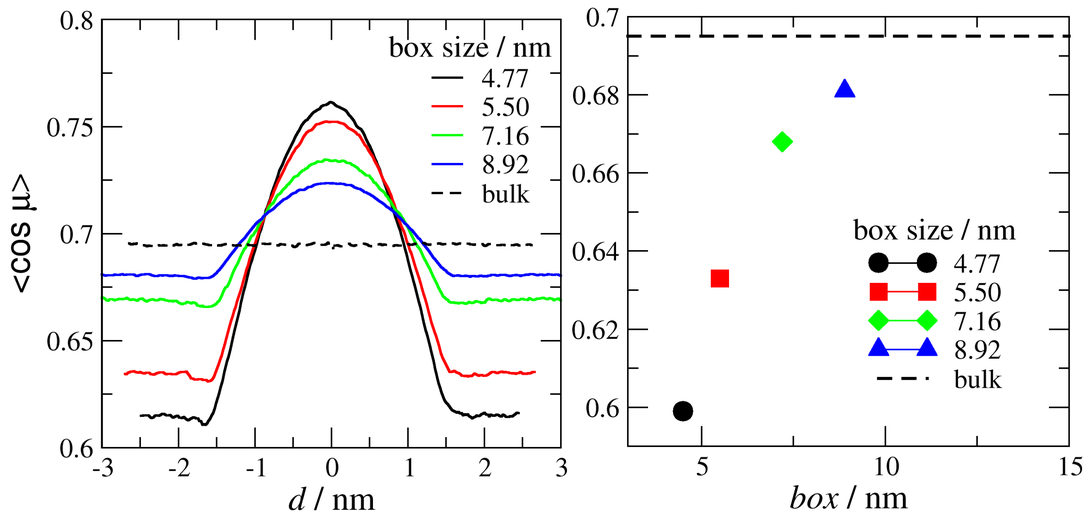




E_x = 0.6 V/nm,
d (box) = 7.2 nm,
T = 300 K

Normalized distributions of calculated migration rates in the direction of the applied electric field (black) and in the non-field directions (blue).

Distribution of mean dipole projections



The average value of the dipole moment projections of water molecules onto the axis of the electric field (left). Surprisingly, the limiting value depends on the size of the simulation box (right).

Conclusions

The observed migration rate of the LJ particle closely resembles the previously reported data for heptane droplets [2]. However, structural properties such as normal correlation functions and average dipole moment projections of water molecules on the axis of the applied electric field suggest that observed electrophoretic mobility may promoted by extremely long range interactions that are induced by the electric field. Currently, the dependence of the observed migration rates on the system size and on the range of van der Waals interactions, are under investigation.

References

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