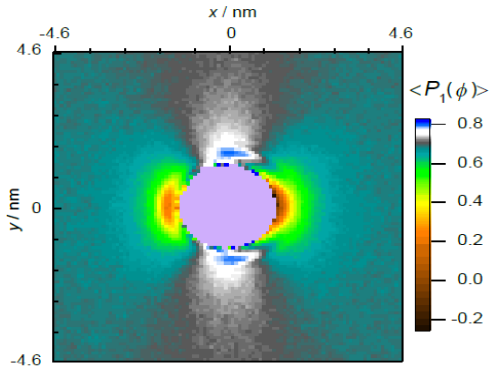
Water ordering around small hydrophobic solutes in electric fields

Z. Miličević[1,2], M. Mališ[3], S. J. Marrink[4], D. M. Smith[2,3], A.-S. Smith[1,2]

[1]Institute for Theoretical Physics, University Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, GERMANY
[2]Excellence Cluster: Engineering of Advanced Materials, University of Erlangen-Nürnberg, Nägelsbachstraße 49b, 91052 Erlangen, GERMANY
[3]Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, CROATIA
[4]Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, 9747 AG Groningen, THE NETHERLANDS

The hydrophobicity of an interface, droplet or a particle can be modulated by an external electric field in a process called electrowetting. [1] Such a change of surface characteristics allows for the regulation of macroscopic properties such as adhesion or friction in micro and nano-fluidics by the electric field. [2] The organization of water around hydrophobic objects, in the absence of an external field, has been studied extensively over the last decades. [3] However, the effect of the field on hydrophobic solvation is much less well understood.

In this contribution, we investigate the detailed structure of water around an idealized hydrophobic solute by means of extensive molecular dynamics simulations. We have used the data from these simulations to evaluate the total solute-solvent correlation function, which includes the orientational degrees of freedom of the solvent. Under the influence of the external field, it is particularly instructive to examine the correlations in the meridian planes of the solute. Similarly revealing is the analogous projection of the water dipoles in the direction of the field (see picture). We find an interesting competition between the optimal orientation of water with respect to the field and the solute particle. On one hand, this results two low-density regions around the +x and –*x* poles of the particle, with the depletion being more pronounced on the +*x* side. On the other hand, the symmetrically placed high-density regions on the +y and –*y* poles appear to have very long-ranged ramifications.



[1] R. Shamai, D. Andelman, B. Berge, R. Hayes, *Soft Matter*, **2008**, *4*, 38-45.

[2] L. Robinson, A. Hentzell, N. D. Robinson, J. Isaksson, M. Berggren, *Lab. On Chip*, **2006**, *6*, 1277-1278.

[3] D. Chandler, *Nature*, **2007**, *445*, 831-832.