Hydration of small hydrophobic objects: The effects of an electric field

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It is well established that the hydrophobicity of an interface, droplet or a particle can be modulated by an external electric field. However, the electric field effects on water structure around a hydrophobic object are not understood to a satisfactorily level. We study the organization of water around a Lennard-Jones particle and an oil droplet in the presence and absence of a static electric field. We perform extensive MD simulations using the GROMACS software package and the SPC/E model of water. The structure of water is analyzed by means of the total solute-solvent correlation function, which includes the orientational degrees of freedom of the solvent. We find that a structure of water arises from the competition between optimal orientation of water with respect to the field and with respect to the solute, yielding an asymmetric distribution of solvent charges around the particle. The particle thus appears a small dipole. Another consequence of the field are very long range solvent-solute effective interactions. We furthermore evaluate the force correlations as a function of time and find them sensitive to the treatment of van der Waals interactions in simulations, which may explain some discrepancies in the observed mobilities of small droplets in simulations reported previously in the literature.