Dielectric behavior of water within a surfactant bilayer: a molecular dynamics study

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Understanding the dielectric behavior of water confined within a surfactant bilayer is essential in the description of different physicochemical processes in biological systems, drug design and enhanced oil recovery, among others. Although extensive work has been done for surfactant and lipid bilayers, less attention has been paid to the dielectric behavior of water confined in it. From the point of view of simulations there is a standard procedure to evaluate the static dielectric constant of a fluid in one-phase simulations, however there are limited attempts to determine the dielectric behavior of water in bilayer geometries. In this work we study the dielectric behavior of water confined between two layers of surfactant. We use four models that have been useful in the description of different properties of liquid water in a wide range of thermodynamic conditions but predict different values of static dielectric constant. The surfactant molecules are described using models proposed in the literature. Our results are discussed in terms of the evaluation of the static dielectric constant of water and structural properties in the bilayer for the SPC/E, TIP4P/2005, TIP4Q and SPCepsilon models. These results are necessary to lay the foundations for a better dielectric characterization of the water contained in films and open the possibility to propose methods that allow the evaluation of these properties when molecular simulations are applied.