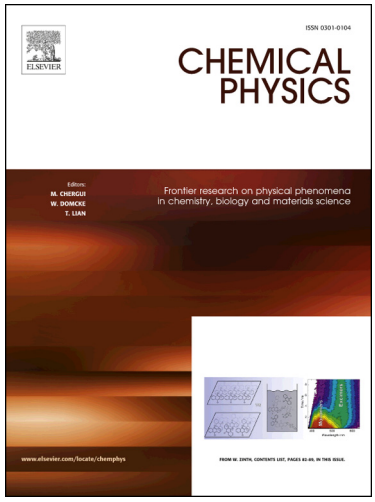

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Chemical potential and free energy of nanoconfined water in Newton black films

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Abstract

In this work we investigate possible approximations to the free energy and chemical potential of water within a Newton black film as a natural nanoconfinement. As a first step we explore the different approximations in a sample of 500 water molecules (bulk water), finding that the overlapping distribution method is the more accurate. For the Newton black film we also calculate the free energy profile of the water molecules along the bilayer normal. We obtain that depending on the position of the water molecule inside the bilayer, the excess chemical potential is lower than that of bulk water, suggesting that a water molecule might be more stable inside the Newton black film than in bulk. A charged semiflexible amphiphilic model and the TIP5P model of water are used in our simulations.

Keywords: Newton black films; TIP5P water; molecular dynamics; free energy; chemical potential

1. Introduction

Thin soap films are simple chemical systems which involve the basic physical interactions existing in more complex structures, like, for instance, biological membranes and foams. In foams, the continuous phase forms thin liquid films, which separate the dispersed gaseous bubbles. The stability of foams depends essentially on the stability of these thin films. Black films, the final stages of the thinning of soap films due to the draining of water in the absence of evaporation, are generally formed from solutions of an ionic surfactant in the presence of a salt. Depending on the salt concentration and the temperature, two different types of black films can be observed: common black films (CBF) with thicknesses $D \sim 10 - 100$nm and Newton black films (NBF) with thicknesses

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