



سمینار هفتگی ماده چگال نرم

Dynamics of Calcium Chloride Aqueous Solutions in Newton Black Films: A Molecular Dynamics Study

Abstract

Water is omnipresent and plays a vital role in countless processes. This strange component is occasionally found at ranges as small as five angstroms. Such systems have been identified as Newton Black Films (NBF) for many years. The behaviour of the free solutions undergoes significant changes in these films. Of course, the presence of soluble salts leads to a more complex behaviour. In this study, we enforced multiple molecular dynamics (MD) simulations to elucidate the dynamics of saline NBFs. We used two flexible water models in the simulations: SPCEF and F3C. We limited the solutions to two layers of n-hexane and considered different contents of calcium chloride (CaCl_2). We then evaluated the dynamics of each system. We found that confinement and salinity restrict the dispersion of all retained particles. However, the reduction of saltiness is weaker in the NBFs compared to free solutions. Moreover, we observed that the dissolved salt implicitly restricts the diffusion of water and hexane. Note that anions diffuse quicker than cations and are more influential. We also obtained water diffusivity as the dominant governing factor in controlling the dynamics of the NBFs. Furthermore, we defined a 'two-phase saturation concentration' around 2M in the NBFs. In closing, we believe this study is a practical step towards understanding the enigmas of Nano-confined aqueous solutions.

Nahid P.Khiabani

Tehran University

زمان: شنبه ۱۳/۱۲/۱۴۰۱ ساعت ۱۵:۳۰

مکان: اتاق ۵۱۲ دانشکده فیزیک دانشگاه صنعتی شریف - کلاس مجازی دکتر اجتهادی

<https://vc.sharif.edu/ch/ejtehadi>