



Absence of image charge effect at hydrophobic interfaces

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日時：2018年2月13日(火) 13:00 – 14:30

場所：ウエスト1号館10階 情報学習プラザ (W1-A-1011)

要旨：

Charged particles like ions or protons at hydrophobic surfaces or at the air-water interface play a major role in a variety of effects like the water surface tension of the electrolyte solution, light particle adhesion or salt effects on bubble coalescence. We study the free energy profile of a single ion at a hydrophobic interface using atomistic molecular dynamics simulations. The interaction of the ion in the vicinity of the surface is dominated by non-electrostatic contributions. To describe the electrostatic part linear dielectric theory is not sufficient, because higher terms are important. To quantitatively explain the linear dielectric contribution we use an anisotropic dielectric model.