Title

The Influence of Confinement on Material Properties and Interfacial Thermodynamics

Abstract

In this presentation, we present the findings of our research projects investigating the effects of confinement on materials properties and interfacial phenomena.

Nanoscale bubbles form when impurities become trapped between a two-dimensional crystal and an atomically smooth substrate. Initially, these bubbles were simply considered as indicators of strong adhesion between the crystals. However, they have since revealed intriguing applications, such as calculating the adhesion energy between two-dimensional materials and investigating the effects of confinement on material properties. These bubbles have previously been observed to conform to a universal aspect ratio (height-to-radius) in their morphology [1]. However, our investigation reveals a departure from this universal scaling when the bubble radius decreases to around 1 nm and below [2]. We interpret this deviation as stemming from the out-of-plane settlements of trapped substances and their atomic compressibility.

Furthermore, nanoindentation of these nanoscale bubbles yields valuable insights, enabling the measurement of the elastic properties of the deformed crystal and the estimation of the hydrostatic pressure within the bubbles. We demonstrate that the failure behavior of nanobubbles under indentation resembles that of viral shells [3] and can be predicted using continuum theories [4]. The confinement induced by the bubbles leads to unexpected thermophysical properties in the trapped substances.

Charged polymers are prevalent in nature and industry. They can be detected, processed, and sequenced by transmitting them inside nanoscale spaces. We investigate how the permeation of charged polymers through nanocapillaries can be modulated by binding counterions. We explain how the surface versus bulk preferences of various alkali cations in small clusters of water, influenced by a strong electric field, impact polymer permeation and transmission speed patterns [5].

Finally, we explore the century-old Kelvin equation, which surprisingly predicts capillary condensation in capillaries as narrow as 1 nm [6], despite its basis in macroscopic thermodynamic homogeneity. We identify inconsistencies within prevailing explanations, proposing a reevaluation through the concept of disjoining pressure. Furthermore, we discuss the breakdown of a previously acknowledged proportionality between the work of adhesion and interfacial thermal conductance [7] in capillaries smaller than 1.3 nm in height, where the dominance of the work of adhesion shifts notably from energy to entropy [8].

References

[1] Nat. Commun. **7**, 12587 (2016).
[2] Nano Lett. **21**, 8103–8110 (2021).

[3] Phys. Rev. Lett. **97**, 228101 (2006).
[4] Nanoscale **14**, 5876– 5883 (2022).
[5] Phys. Rev. E 107, 034501 (2023).
[6] Nature **588**, 250–253 (2020).
[7] Phys. Rev. Lett. **102**, 156101 (2009).
[8] Nano Lett. **24**, 18, 5625–5630 (2024).

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