



THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics

COLLOQUIUM

# Drying and Hydrophobic Collapse of Nanoscale Plates and Protein Complexes

by

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*Date: February 6, 2009 (Friday)*

*Time: 4:30 - 5:30 p.m.*

*Place: L2, Science Centre, CUHK*

*(Light refreshments will be served 20 minutes prior to the colloquium.)*

ALL INTERESTED ARE WELCOME

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## Abstract

My talk will mainly focus on hydrophobic interactions and the water drying transition in nano-scale hydrophobic plates and protein systems. Small solutes can fit into the hydrogen bond network of water without destroying hydrogen bonds, while large solutes have to destroy hydrogen bond network, leading to a dewetting of the hydrophobic surface. The existence of a drying transition for water confined between hydrophobic particles was found to be sensitive to the solute-solvent attractions in molecular dynamics simulations. A drying phenomenon was observed between two paraffin-like plates, but not between two graphite plates. What happens in protein collapse? In the folding of a multi-domain protein, BphC enzyme, no drying transition was observed even at very small inter-domain distances. For example, liquid water persisted with a density only 10 to 15% lower than in the bulk at 4 Angstrom separation of the domains. However, when the attractive forces between protein and water were turned off, a dewetting transition occurred in the inter-domain region and the collapse of the two domains sped up by more than an order of magnitude. On the other hand, the melittin tetramer, displayed a surprising drying transition inside the nanoscale channel formed by the tetramer. To our knowledge, this is the first time a drying transition was found in real protein systems. Surface topology can have significant effects on the drying transition of this system. Single point mutations of the isoleucines in certain locations can switch the channel from being dry to being wet.

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