



THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics

COLLOQUIUM

Characterizing Physical Properties of Nanomaterials: Insights from First-principles Theories

by

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Date: February 19, 2010 (Friday)

Time: 4:00 - 5:00 p.m.

Place: L2, Science Centre, CUHK

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

ALL INTERESTED ARE WELCOME

Abstract

The development of the emerging nanotechnology is ultimately related to the unique physical and chemical properties of nanomaterials. The ability to characterize and predict these properties eventually allows us to modulate and engineer nanomaterials to meet the needs of various applications. First-principles theories, in this regard, can be of great help in interpreting and complementing experimental results, and in developing and validating models. In practice, the predicting power of the theory relies on the accuracy, efficiency, and robustness of the computational tools employed. In this talk, I will demonstrate the importance of first-principle methods with three examples. The first one involves the study of van der Waals interactions in order to predict the microscopic structure of nanomaterials. The second case involves the energy level alignment at the molecule/metal interface in order to predict transport properties of nanoelectronic devices. The last example is related to the optical absorption spectra of nanoclusters, which are of great importance for solar energy applications.