



THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics
Institute of Theoretical Physics

COLLOQUIUM

Multi-Paradigm Simulations at the Nanoscale: Methodology and Applications to Functional Carbon Materials

by

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Date: April 3, 2009 (Friday)

Time: 2:00 - 3:00 p.m.

Place: L2 , Science Centre, CUHK

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

ALL INTERESTED ARE WELCOME

Abstract

Multiparadigm methods to span the scales from quantum mechanics to practical issues of functional nanoassembly and nanofabrication are enabling first principles predictions to guide and complement the experimental developments by designing and optimizing computationally the materials compositions and structures to assemble nanoscale systems with the requisite properties. In this talk, we employ multi-paradigm approaches to investigate functional carbon materials with versatile character, including fullerene, carbon nanotube (CNT), graphene, and related hybrid structures, which have already created an enormous impact on next generation nano devices. The topics will cover the reaction dynamics of C60 dimerization and the more challenging complex tubular fullerene formation process in the peapod structures; the computational design of a new generation of peapod nano-oscillators, the predicted magnetic state in NanoBuds; and opto-electronic properties of graphene nanoribbons.

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