

Physics Colloquium

Michigan Technological University

Thursday, February 26, 2015

4:00 pm

Room 139, Fisher Hall

Novel Two-Dimensional Materials – Boron Nitride Nanomesh & Molybdenum Disulfide Quantum Dots

Jarvis Loh

Department of Physics, Michigan Technological University
Institute of High Performance Computing, A*STAR Singapore

Abstract

It is not an overstatement to claim that graphene has revolutionized and prompted a shift in paradigm in materials research. Indeed, since its discovery a decade ago, immense interest has been generated in other two-dimensional (2D) materials, such as boron nitride (BN) and molybdenum disulfide (MoS_2). In the first part of the talk, a unique form of boron nitride, namely the boron nitride nanomesh, will be introduced, after which the speaker will delineate how this material can be used as a nanotemplate to trap oxygen and hydrogen for novel applications. By using density functional theory, it is demonstrated that the functionality of C doped BN nanomesh can be tailored by an external electric field which modifies the strength of the adsorbate binding to the nanomesh. Specifically, selective binding of H, O, H_2 and O_2 at various sites of the C doped nanomesh – within the pore, on the wire, and at an intermediate site. In the latter part of the talk, the MoS_2 quantum dot (QD) will be examined to investigate the effects of passivation, additional layer, and the h-BN substrate on its geometry, energetics, and electronic properties. The monolayer QD is metallic in nature, mainly due to the coordinatively unsaturated Mo atoms at the edges. A bilayer QD is more stable than its monolayer counterpart. Moreover, substrate-induced modifications in the electronic structure of the quantum dot are not discernible. The metallic character of the QD deposited on the insulating substrate can therefore be exploited to extend the functionality of MoS_2 -based nanostructures in catalysis and electronics applications at the nanoscale level.

Biography



Jarvis Loh, is a recipient of the A*STAR International Fellowship (AIF) in 2013, and is based under the Institute of High Performance Computing (IHPC) in Singapore. As a concurrent appointment, he is deployed as a visiting scientist in the Department of Physics, Michigan Technological University. Previously from 2012-2013, he was a post-doctoral fellow in the Centrale Nationale de la Recherche Scientifique (CNRS), which is the national research organization in France, and the largest fundamental science agency in Europe. Apart from his stint in Europe, he has worked with collaborators from the University of Tokyo, Rice University, and his alma mater, Nanyang Technological University.

He earned his B. Eng. (1st Class Hon., Accelerated) and Ph.D., both in electrical and electronic engineering from Nanyang Technological University in 2008 and 2012 respectively. His research interests include the computational (first-principles and atomistic) and theoretical modeling of thermal transport phenomena, thermoelectrics, phase transformation, and electronic properties of nanomaterials. He has published more than 20 peer-reviewed scientific articles in reputable journals such as *Advanced Materials*, *Applied Physics Letters*, *Journal of Applied Physics*, *Journal of Materials Chemistry C*, and *Journal of Physical Chemistry C*.

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