



## *Molecular Dynamic study of Diffusion of C60 on Graphene Substrate*

by Mr. Mehdi Jafary Zadeh

**Date:** 12<sup>th</sup> November 2009 (Thursday)  
**Time:** 12:00pm to 12:30pm  
**Venue:** EA-02-11 (Executive Seminar Room)

### Abstract

Surface diffusion and diffusive properties of adatoms and ad molecules on different substrates are fundamental phenomena for better understanding of many interesting concepts in science and technology such as nanostructuring, crystal and film growth, catalysis, phase transformations, surface reactions and all other types of surface processes. After advent of some advanced experimental techniques such as STM, QHAS and optical diffraction grating, it is possible to directly measure the surface diffusion coefficient of many systems. However, these methods are not applicable in all substrates and usually it is only possible to study few snapshots of the diffusing particle movement. On the other hand, using numerical and simulation tools, it is possible to study the step-by-step movements of a diffusion system and have a detail analysis of the mechanism.

In the current research Molecular Dynamics, which is consisted of numerical solution of Newton's equations of motions for all atoms in the system, has been used to study the diffusion mechanism of C60 ad molecule on the graphene substrate. The interesting issues to be addressed in the selected system are estimation of the diffusion prefactor and energy barrier based on Arrhenian analysis. Moreover, the internal degree of freedom of C60 ad molecule and its effect on diffusion behavior and mechanics of motion is of interest.

**Mr. Mehdi Jafary Zadeh Speaker**

Mr. Mehdi Jafary Zadeh, obtained his B.Sc. in "Industrial Metallurgy" in 2000 from Isfahan University of Technology, Isfahan, Iran. Later, he obtained his M.Sc. in Materials Science and Engineering in 2002 from "Sharif University of Technology", Tehran, Iran. He is now a PhD candidate in Department of Materials Science and Engineering, NUS since 2008, and according to his interest in computational materials science, doing his research under the supervision of Prof. Zhang Yang-Wei in the field of Molecular Dynamics Simulation.

**Dr Xue Jun Min Host**

*All are Welcome!*