Physics Colloquium

Michigan Technological University

Thursday, January 27, 2011, 4:00 pm

Room 139, Fisher Hall

Interaction of Nanomaterials with Biological Molecules : Manganese and Dopamine

Chunhui Liu

Advisor: Dr. Ravi Pandey

Abstract: We present the results of our *first-principles* quantum mechanical calculations describing the interaction of metallic nanoparticles (NPs) with biologically active molecule, dopamine. The metallic nanoparticles are represented by Mn_{13}, Ag_{13} and Al_{13} atomic clusters. Our calculations suggest that the interaction is governed by the strength of the covalent bonds between the atoms in nanoparticles and the organic molecule. The interaction strength, determined in terms of the nanoparticles-molecule binding energy, is found to be higher for Mn clusters than the Ag and Al clusters. Furthermore, the NP-molecule binding energy strongly depends on the angle of approach of the two systems, suggesting site specificity of the NP-molecule interaction. The results, which form the basis of a comprehensive kinetic model describing the NP-molecule reactivity, may also explain the observation of different levels of dopamine depletion in PC-12 due to the presence of Mn and Ag nanoparticles in an experimental study (Toxico. Sci. 92, 456, 2006).

First Principles Study of Strain Induced Modulation of Energy Gaps of Graphene/BN and BN Bilayers

Xiaoliang Zhong

Advisor: Dr. Ravi Pandey

Abstract: First-principles calculations based on density functional theory are performed on graphene/BN and BN bilayers to investigate the effect of the pressure which is perpendicular to the bilayer system on their energy gaps. For the graphene/BN bilayer, the bands have characteristic graphene-like features with a small band gap at K. Application of pressure modulates the band gap whose magnitude depends on the strength of interaction between constituent monolayers. For the BN bilayer, on the other hand, a large band gap is predicted which remains nearly the same for small strains. The increased inhomogeneity in charge density of different carbon sublattices due to a stronger interplanar interaction is the cause of the predicted variation in the band gap with strains applied along the perpendicular direction in the graphene/BN bilayer.

Kinetic Monte Carlo and Master Equation Approaches To Solving a System of Rates

Douglas Banyai

Advisor: Dr. John Jaszczak

Abstract: Last week we saw Partha and Saikat characterize the transport properties of molecular junctions from first principles. This week I will describe ways to calculate the transport properties of a class of systems that contain multiple such junctions and are too big for an ab initio treatment. We will look at a specific condition under which the standard methods for finding a Thevenin equivalent for the system fails, and introduce a semi-classical model to account for the differences. This model will allow us to calculate the rates at which we expect electrons to traverse individual junctions, but these rates need to be integrated to find the current through the entire device. Kinetic Monte Carlo and the master equation approach are two ways to do this.

A master equation (ME) describes how the probability for a system to be in a given state changes in time. In certain simple systems, the steady state solution can be found very efficiently and from this, properties of the system can be calculated. Kinetic Monte Carlo (KMC) is a powerful method for calculating both transient and steady state properties, and can handle more complex systems than the ME method. I will describe the theory and implementation of both the ME and KMC algorithms, and show example results from a toy model.

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