

# Physics Colloquium

## Michigan Technological University

Thursday, January 20, 2011, 4:00 pm

Room 139, Fisher Hall

### **Ab Initio Study of Electron Transport in Strongly Coupled Molecular Junctions**

**Partha Pal**

**Advisor: Dr. Ranjit Pati**

**Abstract:** In this talk, I will report a first principles study on the evolution of charge transport in a two-terminal molecular scale device consisting of a molecular nanowire sandwiched between two Gold electrodes. The molecular wire is built out of a series of bicyclo[1.1.1]pentane (BCP) oligomers. The length of the wire ( $L$ ) is increased by sequentially increasing the number of BCP cage-units in the wire from 1 to 3. A parameter-free, non-equilibrium Green's function approach is used to study the current-voltage characteristics of each of the devices. In the low bias regime, the current-voltage characteristics are found to follow Ohm's law in all the three devices. However, the conductance ( $G_C$ ) of the nanowires is found to decrease exponentially with increase in length following the relation  $G_C = G_0 e^{-\beta L}$ . This is in excellent agreement with the earlier reported exponential decay feature of the electron transfer rate predicted from the electron transfer coupling matrix values obtained using the two-state Marcus-Hush model and the Koopman's theorem approximation on the same system. The downright suppression of the computed electrical current for a bias up to 0.4 V in the longest wire can be exploited in designing a three terminal molecular transistor; this molecular wire could potentially be used as a throttle to avoid leakage gate current.

### **Colossal Conformational Gating in a Molecular Three-Terminal Device**

**Saikat Mukhopadhyay**

**Advisor: Dr. Ravi Pandey**

**Abstract:** The effect of conformational changes in the gate arm of a three terminal molecular device is investigated. Two donor-acceptor substituted  $\pi$ -conjugated molecular moieties joined by a phenyl ring junction describe the two arms, whereas a triphenyl molecular wire, also connected to the junction ring serves as the gate arm in the proposed architecture. In the ground state equilibrium geometry, the gate (triphenyl) arm is non-planar, where the middle phenyl ring is approximately  $30^\circ$  out of plane with respect to other two rings. At this geometry, the calculated tunnel current ( $I_d$ ) as a function of applied external bias ( $V_{ds}$ ) across the two D-A substituted arms exhibits a typical insulator-semiconductor behavior. Similar  $I_d$ - $V_{ds}$  characteristics is calculated when planarity of the triphenyl arm is restored. However, a colossal increase, by more than an order of magnitude, and a sharp rise in the current are predicted when additional non-planarity, by  $30^\circ$  is induced in the triphenyl chain. Analysis of the results suggest that, unlike in "voltage" gating, neither the HOMO-LUMO gap nor the dipole moment of the system undergo significant changes due to pure conformational gating as observed in this study. Instead, the observed conformational gating affects the current via localization/delocalization of the electronic wave function in the conduction channel. Furthermore, the tunneling current corresponding to conformational gating in two different directions appears to exhibit oscillatory nature with a phase factor of  $\pi/2$  in presence of the gate field. The current modulation is found to reach its maximum only under exclusive effect of voltage or conformational gating and diminishes when both of them are present.