Physical Chemistry Seminar

Tuesday, November 6, 2012 | **11:00 am** | **Room 1315 Chemistry Building**

Computational studies of energy transfer in dendrimers

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Host: Professor Ned Sibert

Excited state nonadiabatic molecular dynamics simulations are used to study the nature of the energy transfer in different model dendritic molecules built from linear poly-phenylene ethynylene (PPE) in different architectures. Dendrimers built from these building blocks have been experimentally shown to undergo highly efficient and ultrafast unidirectional energy transfer. We have recently introduced a highly efficient method to compute non- adiabatic excited-state dynamics, including analytically computed gradients and non- adiabatic couplings.The simulations start by an initial vertical excitation selected according to the experimental conditions. By running many simulations, we observe ultrafast and mostly one-directional electronic energy transfer, concomitant with an also ultrafast vibrational energy transfer. The energy gaps and nonadiabatic couplings are strongly influenced by the different nuclear motions in the different potential energy surfaces. This behavior guarantees the successful unidirectional energy transfer associated to the efficient energy funneling in light-harvesting dendrimers.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335