

# Physics Colloquium

Michigan Technological University

Thursday, March 4, 2010

4:00 - 5:00 pm

Room 139, Fisher Hall

## Calculation of Optical Properties for Molecular-to-nanomaterials

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**Abstract:** To calculate photophysical properties of materials that exhibit multiphoton absorption, validation of density functional theory (DFT)/time-dependent DFT (TDDFT) for chromophores of interest is discussed, in particular the use of an appropriate exchange-correlation functional, for investigating charge-transfer excited states. In new directions, photophysical properties of nanoscale clusters that exhibit two-photon absorption (TPA) are described, specifically regarding gold and semiconductor nanoclusters. Aspects relating to the structure, one-photon (OPA) and TPA spectra prediction of stable “magic-size”  $[\text{Au}_{25}(\text{SR})_{18}]^{-1}$ , gaining insight into the large experimentally observed TPA, are discussed, as well as OPA for small stable CdSe nanoclusters of varying size. Finally, the possible utility of plasmonic Au nanorods is reported. In this context, computational prediction of fluorescence enhancement and quenching by simulation of emitters proximate to metal nanoparticles is summarized.

**Biography:** Dr. Ruth Pachter is a Senior Scientist, Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base. Dr. Pachter, a member of the scientific and professional cadre of senior executives, was appointed a senior scientist in 2001. She joined the Materials Directorate in 1991, from Stanford University, where she conducted research in the Biophysics Program. In 1994, she was appointed a physical scientist at the National Institute of Standards and Technology, co-located at Wright Laboratory, and in 1997 became a principal physical scientist in AFRL. Dr. Pachter received her undergraduate degree in Chemistry and Physics from the Hebrew University, Israel, and her graduate education in Theoretical Chemistry from the Technion, Israel Institute of Technology, and the University of South Africa. Dr. Pachter’s research interests span a wide range of theoretical studies of molecular-to-bio/nanoscale materials for Air Force applications.