Department of Mathematical Sciences Colloquium

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Application of Density Functional Theory to Light-Harvesting Molecular System

Density functional theory (DFT) has emerged as a powerful computational tool for studying the electronic structure of a vast array of systems ranging from atoms to solids. It has an advantage over the higher level quantum chemistry methods in that it can handle larger systems with a relatively smaller price for accuracy. In this talk I present some applications of DFT for a large molecular composite system which can be used as a molecular level photovoltaic. Such study requires a good understanding of excited states. I will talk about a new computationally low-cost DFT method being developed by us for treating the excited states and its application to a light harvesting molecule.

Friday, April 7, 2006 at 3 pm in Bell Hall 143
The University of Texas at El Paso

Refreshments will be served in front of the colloquium room, 15 minutes before the start of the colloquium.

For further information, please contact Dr. Pavel Šolín, Bell Hall 220. Phone: (915) 747-6770, email: `solin@utep.edu`.