Modeling of Solvent Electrostatic Effects

Jose A. Rodriguez Lopez^  
*Department of Physics, University of Texas at El Paso, tonymax90@hotmail.com

Luis Basurto  
*Department of Physics, University of Texas at El Paso, lbasurto3@utep.edu

Tunna Baruah*  
*Department of Physics, University of Texas at El Paso, tbaruah@utep.edu

Follow this and additional works at: http://digitalcommons.utep.edu/couri_abstracts

Recommended Citation  
http://digitalcommons.utep.edu/couri_abstracts/42

This Article is brought to you for free and open access by the COURI Symposium Abstracts at DigitalCommons@UTEP. It has been accepted for inclusion in COURI Symposium Abstracts, Spring 2011 by an authorized administrator of DigitalCommons@UTEP. For more information, please contact lweber@utep.edu.
Modeling of Solvent Electrostatic Effects

José A. Rodríguez López^, Luis Basurto, Tunna Baruah*

Department of Physics, University of Texas at El Paso

The photo-induced charge-transfer process is fundamental to light harvesting in organic donor-acceptor systems. The process is often enhanced when the system is in a polar solvent. The aim of this project is to create a simple, discrete model containing dipoles that can explain the solvent effects, where only dipole-dipole solvent interaction is considered. The goal is to reduce computational complexities and cost. We create a grid of solvents (water) which mimic the solvent’s density; and put one solute (a light-harvesting triad of β-carotene, porphyrin, and C60) at the grid’s center, keeping the grid points 1.5 times the Van der Waal radii away from the solute atoms. The solute’s partial charges and the solvents dipoles create an electrostatic field which determines the solvent configurations. Using Monte-Carlo method and classical electrostatics at a given temperature we obtain the lowest energy and the average configuration of the grid. Our calculations are performed at T=300K and T=10K for the ground and charge-transfer excited states of the solute. The field due to the solvents can be used in quantum mechanical calculations to determine the solvent effects. Future work will include the induced dipole moments of the solvents into the calculation and also use a variable grid.