

Statement of Research Interests

Volkan Ediz

Previous Research experience

- Synthesis of model polydimethylsiloxane and polyether based segmented polyurethane and polyurea copolymers and investigation of their structure-property relations. (2002)
- Understanding the hydrogen bonding in metal salt doped polyurethanes: Quantum mechanical studies were used to explore the effects of hydrogen bonding on the IR spectra, allowing structural information to be obtained from such spectra on dimethylurea blends doped with transition metal salts CoCl_2 , FeCl_3 , and LiCl . (2003)
- Modeling the electronic properties of cyanine dyes used in bio-imaging: Semi-empirical quantum chemistry methods revealed a thermally activated transition from the planar to twisted geometry that could account for observed substituents effects on the fluorescence quantum yield in solution and account for the large change in quantum yield seen on binding to DNA. (2005)

Current Research

Experimental studies of the optical properties of single-walled carbon nanotubes (SWCNT) have recently generated considerable experimental and theoretical interest. Smalley et. al. showed that mapping of optical transitions to (n,m) numbers that characterize a nanotube provides an empirical rule which can be used for structure assignments. There is growing agreement that the optical excitations correspond to bound electron-hole pairs, or excitons, but the details of these exciton states are still under debate. My goal is to better understand the nature of these excitations in different types of semiconducting tubes, by comparing the electronic spectra of tubes at three levels of theory [Huckel, Pariser-Parr-Pople (PPP) and Intermediate Neglect of Differential Overlap (INDO)]. This should allow me to unravel the influence of the various factors (band structure and curvature, electron-hole binding potential) on the excitons and better understand how the excitonic spectra arise from the tube structure (n,m). An important aspect of the project is optimizing existing methods, by using direct configuration interaction approaches, such that periodic boundary condition calculations can be done rapidly on large structures.

Reason for participation in the ICYS-ICMR Summer School

By interacting with new colleagues who shares similar research interests, I hope to broaden my current knowledge of nanotechnology and gain a better understanding of how computational chemistry can contribute to this field.

Publications

Silva, G., Armitage, B., Yaron, D., Ediz, V., Fluorinated cyanine dyes for detection of DNA (in preparation)

Ediz, V., Yaron, D., Computational studies of excitons in carbon nanotubes. Abstract of Papers, 232nd ACS National Meeting, San Francisco, CA, United States, September 10-14, 2006 (submitted)

Yilgor, I., Atilla, G. E., Ediz, V., Yilgor, E., Yurtsever, E., Understanding the hydrogen bonding in polyurethanes: Quantum mechanical calculations and experimental studies on model systems. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003