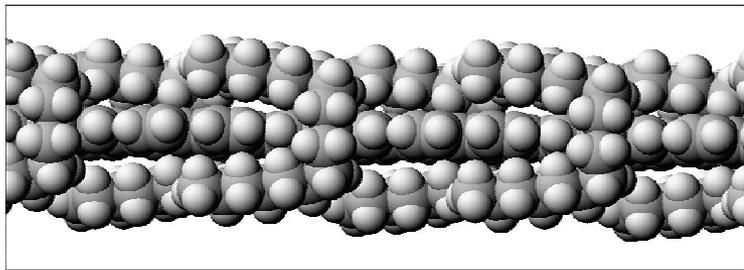


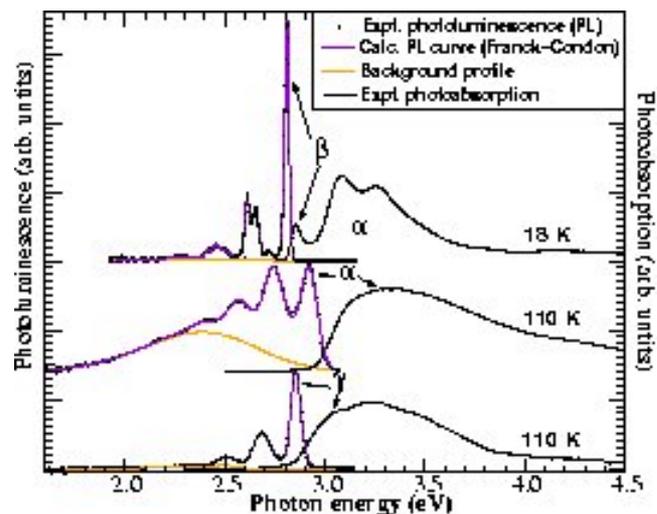
Molecular-Level Studies of Structure and Photophysics in Conjugated Polymers

Michael J Winokur, University of Wisconsin, DMR-0350383

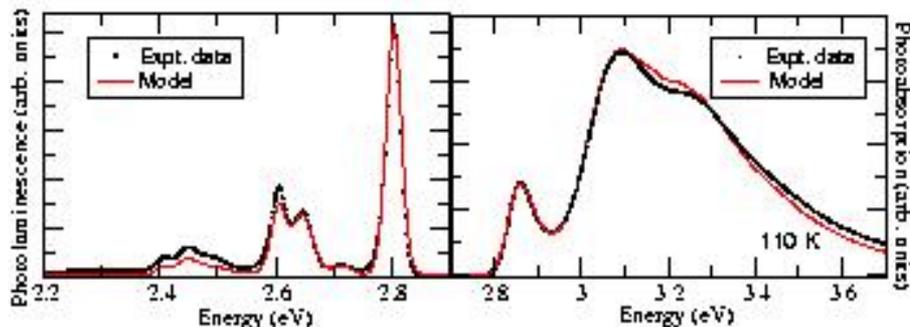
Explicit knowledge of the molecular-level structure and structure/property relationships in electronic polymers is essential for establishing a fundamental understanding of both the charge transport and photophysics. This information is also centrally important for new device technologies incorporating these unique materials. This research examines the underlying structure and structural phase behavior in these polymers and then uses this information to develop explicit molecular models. Here we present recent results that identify key relationships between various single chain conformational structures and the diverse optical properties seen in poly(*di-n* octylfluorene) (PF8), a technologically important blue-emitting π -conjugated polymer.



Molecular model of the proposed near-planar β type conformational isomer.



Combination photoluminescence/photoabsorption spectra from three PF8 polymer thin film samples demonstrating the existence of three distinct conformational isomer families (α , β and γ). The β type “family” consists of just a single isomer.



Single-band exciton model calculation of PF8 photoabsorption and photoluminescence (includes Franck-Condon vibronic progression) for a thin-film sample containing an admixture of α and β type conformers.

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Education:

This grant currently supports two students that are completing their Ph.D. degrees: Withoon Chunwachirasiri (graduating in Fall 04) and Boy Tanto (2nd year student). In addition a gifted high-school student, Beau Lynn-Miller, is being supported to work on a project in collaboration with Prof. Paul Evans (UW-Materials Science). This grant has also provided partial support for a graduate student Hyunseok Cheun. The grant also facilitates collaborative research conducted by a graduate student, Jason Slinker (at Cornell University in the group of George Malliaras) and by Brad Larson (at UW-Madison in the group of Max Lagally)

Outreach:

Every spring semester one or two freshman undergraduates (enrolled in an honors introductory chemistry course) are engaged in short term research projects under supervision of the NSF supported graduate students. The group also maintains a web page, at <http://romano.physics.wisc.edu>, that provides resource information and conjugated polymer tutorials.