



# SEMINAR SERIES 2019

Monday, March 25

3:00 pm

1008B Digital Media Center  
Louisiana State University



*Guest Speaker*

**Dr. Lilo  
Pozzo**

The Weyerhaeuser  
Endowed Associate  
Professor of  
Chemical  
Engineering

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Washington

Conjugated polymer films, nanofibers, and networks can be ideal materials for the design of efficient photovoltaic devices, batteries, thermoelectric cells, light emitting diodes and many emerging energy technologies. It is also recognized that the structure and dynamics of organic semiconductor materials correlates strongly with large changes in optical, electronic and mechanical properties so that their control and manipulation is essential to advancing the field. This presentation outlines the use of neutron scattering techniques in the development of structure-property relationships for conjugated polymer nanomaterials. It also highlights recent results on the use of neutron and x-ray scattering techniques for improvements in molecular simulation force fields specifically produced for conjugated polymers. Quasi-elastic neutron scattering (QENS) experiments are used along with computationally efficient MD simulations to understand the nature of important nanoscale motions. X-ray and polarized neutron diffraction are also used to correlate experimental and model-generated polymer structures. QENS validation of MD force fields presents a unique opportunity to increase the accuracy of highly uncertain parameters used in simulation of conjugated polymers and other complex macromolecules. These parameters are currently estimated from quantum mechanical calculations such as density functional theory but, unlike many force fields for small molecules, they are not parameterized to available experimental data. Moreover, high variability is observed in parameters for the small number of force fields that have been proposed in the literature.

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