ACADEMY OF DISTINGUISHED RESEARCHERS

Guest Lecture

Friday, October 20, 2017 | 4:00-5:00 PM
JPL Assembly Room (JPL 4.04.22)

Networking reception with light refreshments to follow.

Translating the Message in Spectroscopic Probes of Conjugated Molecular Materials

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Since before the award of the Nobel Prize, 17 years ago, to Alan J. Heeger, Alan G. MacDiarmid and Hideki Shirakawa for the discovery of conducting polymers, their has been a steady increase in investigations of related electronically conjugated materials for use in solar photovoltaic cells, organic light emitting diodes, and organic material transistors. While the challenges in developing organic LEDs have been overcome and these materials now play an increasing role in commercial products, the progress in the other arenas, using semiconducting polymers, has been steady but slower. A major reason is a fundamental lack of knowledge about the nanoscale organizational structure underlying variations in electro-optical behavior in these typically amorphous materials. Hence, in contrast to familiar silicon-based technology, there is a dearth of principles needed to drive the bottom-up design of new molecular material building blocks.

In the laboratory, scientists most readily probe materials by its response to light, i.e., spectroscopically. The challenge then is to interpret the observations in physical and structural terms. Computational modeling based on the physics of atomistic details and explicit electronic structure is ideally suited to enabling this connection of spectra to structure, since the connection in modeling is unambiguous while the experiment provides a strong constraint on the validity of the model. In this presentation, I will discuss examples of conjugated molecular material systems studied by a coordinated theoretical, modeling, and experimental approach that elucidates both atomistic and electronic structure and dynamics in a way inaccessible to either theory or experiment alone.

Peter J. Rossky is Dean of Rice University's Wiess School of Natural Sciences, Harry C. & Olga K. Wiess Professor of Chemistry and Professor of Chemical and Biomolecular Engineering. Rossky is a leader in theoretical chemical physics and has contributed in the fields of biophysical chemistry, solution chemistry, and molecular spectroscopy, with emphasis on elucidation of the molecular-level description of condensed phase chemical processes in solutions and amorphous materials. He is a National Academy of Sciences member, an American Academy of Arts and Sciences member and a fellow of the American Association for the Advancement of Science. He received his Ph.D. and M.A. in Chemical Physics from Harvard University and his B.A. in Chemistry from Cornell University.

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