## 第638回 化学・物質工学セミナー

## Planar waveguide ATR spectroscopy in the frequency and time domains: Development and application to photochemical and electrochemical reactions in molecular films

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総合教育研究棟 多目的ホール

S. Scott Saavedra教授は、固体/液体界面及び生体分子や超分子などの薄膜の構造に関し、電気化学的手法と分光化学的手法を組み合わせた解析的な研究を精力的に進められておられます。特に、電極表面などにおける微量の生体関連物質の構造と機能を、光導波路を用いてアプローチする研究では世界の第一人者です。今回の講演では*in situ*分光解析に関する研究成果を中心に講演をいただく予定です。奮ってご参加ください。

なお、本講演は、工学研究科グリーンシステム創成科学専攻の講義「国際セミナー」を兼ねます。

## **Abstract**

This talk will describe a novel form of electroreflectance spectroscopy, potential-modulated, attenuated total reflection spectroscopy (PM-ATR). In PM-ATR, the intensity of visible light propagating in a planar waveguide coated with indium-tin oxide (ITO) is monitored while an ac potential modulation is simultaneously applied to the ITO layer. The evanescent field at the surface of the waveguide interacts with an overlying thin film of redox-active chromophores. Changes in the absorbance of the film as a function of the light polarization, modulation frequency, and amplitude provide information about electron transfer rates and molecular structure. We are using PM-ATR to study the relationship between electrochemical kinetics and molecular orientation in monolayers of organic chromophores tethered to ITO, where the monolayer is a model for the first donor layer in a organic photovoltaic (OPV) device. Charge transfer efficiency at the organic/electrode interfaces in OPVs can be an important parameter in overall device performance. Rates of charge transfer across these interfaces are determined by a number of factors, such as offsets in frontier orbital energies, wave function overlap, reorganization energies, and charge mobilities, which in turn depend on structural parameters, e.g. packing and orientation, of the interfacial molecular layers. Modification of the ITO/donor interface with a redox-active, organic surface modifier may enhance charge injection across the interface by providing a facile electron transfer pathway between the contact and the adjacent organic layer, and by controlling chemical and physical interfacial compatibility and the effective work function of the contact.

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