The Department of Chemistry and Biochemistry

Seminar Series

Presents a Seminar Titled:

"Novel Algorithms and Instrumentation for Vibrational Spectroscopic Methods of Analysis"

Presented By

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Raman spectroscopy is a form of vibrational spectroscopy that has been increasingly applied to qualitative analysis of chemicals, explosives, pharmaceuticals, and fuels due to its non-invasive and non-destructive nature; its ease of sampling; and its high molecular specificity. These characteristics of Raman spectroscopy also facilitate its use for both in-line and at-line analysis. The principle limitation of Raman spectroscopy is optical interference arising from both analyte and non-analyte fluorescence. In this dissertation, a solution to this problem is presented in the form of a novel spectrometer design which operates in a sequentially shifted excitation mode to eliminate fluorescence backgrounds, fixed pattern noise, and room lights, while keeping the Raman data in true spectral space. The Raman data is extracted from the shifted excitation spectra using a novel algorithm which is three orders of magnitude faster than conventional iterative algorithms. The superiority of the instrument and algorithm is demonstrated by comparison to FT-Raman, standard deviation spectra, SERDS, and conventional multiple-shift excitation methods.

Near infrared spectroscopy is another form of vibrational spectroscopy which has also been increasingly used for the analysis of fuels in both at-line and in-line applications. Despite its popularity, near infrared spectroscopy lacks the spectral resolution of Raman spectroscopy and because of this, the transfer of quantitative calibration models is considered extremely difficult and expensive. This is considered one of the principle limitations in the use of near infrared spectroscopy for fuel analysis. In this dissertation, a solution to this problem is presented in the form of novel calibration transfer algorithms which allow the use of virtual fuels which are digitally synthesized from pure chemical standards, to transfer quantitative calibration models between different near infrared instruments. This solution eliminates the expense, time, and difficulty of traditional calibration transfer methods."

Friday, March 22, 2013 at 11:00 in Alfriend 111