Analytical Seminar

Thursday, Sept. 16

Room 1315 Chemistry

Professor Peter Chen

Dept. of Chemistry, Spelman College

High Resolution Coherent 2D Spectroscopy of Molecules that Resist Analysis

Coherent multidimensional spectroscopy is an emerging field that provides new capabilities beyond that of traditional one-dimensional spectroscopies. Like 2D NMR, coherent 2D spectroscopy can be used to improve spectral resolution, reduce congestion, and extract new information related to molecular structure and behavior. This talk focuses on the development of high resolution coherent 2D spectroscopy as a new spectroscopic tool for studying heavily congested electronic spectra of gas phase molecules that have long frustrated spectroscopists. Nitrogen dioxide plays an important role in atmospheric chemistry, and its spectrum has been studied for more than 150 years. However, the vast majority of the NO_2 electronic spectrum has resisted analysis. The primary reason for this difficulty is the molecule's unusual behavior due to a series of conical intersections. The resulting spectrum has a reputation of being one of the most difficult to interpret; for example, its unusually dense and broad absorption profile is extremely congested and appears to lack regular repeating patterns. The apparent lack of patterns makes it difficult to use conventional analysis and fitting techniques that rely heavily on pattern-recognition. However, high resolution coherent 2D spectra of NO_2 appear very different; although they still contain a huge number of peaks (tens of thousands to millions) that are sometimes heavily congested, they also contain numerous repeating patterns. New two-dimensional tools (e.g., specialized 2D filters and multi-cluster analysis) are being developed and tested in order to facilitate analysis of the resulting 2D patterns and peak assignment.