**CHEM 7520 Topics in physical chemistry**

**Vibrational spectroscopy: advanced applications for biomaterials**

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**Content**: Vibrational spectroscopy in all its forms - IR, Raman and many variations – is gaining increasing importance in biological and clinical sciences; see, for example, the recently inaugurated International Society for Clinical Spectroscopy (<http://clirspec.org/>) and Raman4Clinics (<https://www.raman4clinics.eu/>). Other biological applications range from the study of aquatic organisms e.g. diatoms, to water quality parameters and food preparation. The majority of macromolecular vibrational spectroscopy requires a sound understanding of the different spectroscopic techniques and the resulting data; spectral bands and the basis of functional group analyses, both the strengths and the limitations are of paramount importance.

The course will begin with a brief introduction and review of the theoretical basis for the normal mode description of vibrations, with examples of computational modeling of small to medium sized molecules to illustrate and contrast different levels of theory used in describing normal modes energies as well as response to polarized light. Students will learn instrumentation design principles and advanced ancillary techniques appropriate for different types of research applications. Topics to be covered include the mathematics of the Fourier transform as implemented in an FTIR interferometer, and the dispersion methods required for Raman spectroscopy. Options for pre- and post-processing of data, such as apodization functions, noise reduction, Fourier self-deconvolution and derivatives will be examined and tested on real spectra, using the software associated with the in-house equipment [FTIR (Agilent) and Raman (Renishaw) research microscopes]. Basic uni-variate and multi-variate statistical approaches will be considered for evaluation of masses of data, such as those arising from large area imaging or from large sample numbers, as well as spectral and spatial resolution, and noise reduction.

Notable advances in instrumentation for FTIR and Raman in the past 10 years have led from micro to to nano-scale capability, mainly via AFM-style tip enhancement combined with lasers: single frequency and tunable Quantum Cascade Lasers (QCL) or broad band lasers of different types (OPO, DFG). Attenuated Total Reflectance FTIR, nano-scale near-field infrared spectroscopy and imaging; time-dependent FTIR to reveal monitor folding dynamics, Resonance Raman, Surface Enhanced Raman and Tip Enhanced Raman, will form the basis of later seminar and student presentations (Powerpoint talks, about 30-40 minute presentation, with questions to follow in class). Areas of application include biospectroscopy, micro and nanoscale imaging. Depending on class interest, additional topics could include material science, polymer science, films, etc. Current literature will be a primary resource, along with texts on theory and instrumentation and relevant web-based sources.

**Evaluation**: This is run in multiple formats with about 50% of the time being spent in lecture/discussion mode, 30% in student-led seminar presentation & discussion and 20% in hands-on activities. Students will be evaluated on participation in discussions, presentations and laboratory-based assignments, and a final exam.