Calculation of vibrational spectra of molecules based on the Raman effect

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Electronic and vibrational spectroscopies are useful tools to provide information on structures and properties of molecular systems. Therefore, an accurate simulation of the spectra of molecules, using quantum chemistry methods, can help in the interpretation of experimental data as well as in the design of new compounds for specific applications, e.g., in molecular sensing, in photocatalysis or in solar energy conversion.
In this talk, I will review some of our results obtained in the simulation of resonance Raman spectra of organic compounds and of ruthenium transition metal complexes. Then, I will present an application of the IR/Visible sum-frequency generation spectroscopy to determine the molecular orientation in self-assembled monolayers. In the last part, I will show some of our recent investigations concerning BODIPY-based sensitizers and their application in triplet-triplet annihilation up-conversion.