**COMPUTATIONAL SPECTROSCOPY: FROM ASTROCHEMISTRY TO BIOMOLECULES**

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Detection of simplest organic molecules in the interstellar space (ISM), prebiotic molecules evolution toward more complex species and biomolecules self-assembly and structure-function relations are nowadays studied by spectroscopic techniques. The focus of this talk is on vibrational “fingerprints” in the ground electronic states, which call for accurate and reliable theoretical support in order to link the rich experimental data to the desired information on the structure and properties of complex molecular systems.

In this respect gas phase experiments allow analysis of unperturbed molecular systems, and are also of direct relevance for the detection of molecules in astrochemical environments. For the latter importance of vibrational spectra shall greatly increase in the future thanks to the MidInfrared Instrument (MIRI), part of the James Webb Space Telescope (JWST), to be launched in 2020. Considering other, more complex systems fingerprint vibrations are influenced by a 3-D structures, and are very sensitive to the weak inter- and intra-molecular interactions, causing band shifts and significant intensity variations.

I will present status and perspectives of the ongoing project aiming to bridge the gap between sophisticated experimental techniques and often over-simplified analysis characterised by low precision and high risk of biased interpretation. Moving toward first principle based anharmonic methodologies, which cover the most important vibrational fingerprints, will significantly improve level of accuracy and understanding of state-of-the-art contemporary spectroscopic results.

In this respect density functional theory (DFT) is nowadays a method of choice for theoretical studies of medium-to-large molecular systems. However, application of DFT to computational spectroscopy imposes additional requirements on the accuracy of DFT functionals, these are the accurate predictions of (i) equilibrium molecular structures, (ii) free energies of different conformers for specific experimental conditions, and (iii) harmonic and anharmonic vibrational properties. Improved accuracy can be achieved by hybrid models, which combine an evaluation of the equilibrium structure, as well as of the harmonic PES and PS, at the highest possible level with anharmonic corrections computed by means of less expensive techniques. In particular, we are employing CC/DFT approach defined by the combination of CCSD(T) (including composite schemes) with DFT functionals.

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