

# Vibrational non-harmonicity effects on the spectroscopy of medium sized molecules and nano structures

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## Organisers

- Majdi HOCHLAF (University Paris-Est, France)
- David LAUVERGNAT (University Paris-Sud, France)
- Roberto LINGUERRI (University Marne-la-Vallée, France)

## Introduction and motivation

The recent developments in the field of vibrational molecular spectroscopy and dynamics allow for the description of isolated medium- and large-sized molecules and nano structures with methods of quantum chemistry based on the harmonic approximation. The main topic of this workshop concerns the development of new methods in order to go beyond the harmonic approximation via the inclusion of non-harmonic effects in molecular dynamics and spectroscopy. Applications include accurate description of weakly bound isolated molecules (e.g. bases pairing in DNA), and molecules physisorbed on grapheme and graphitic nanostructures. It will allow for solving still unanswered challenging problems on molecular physics.

## State-of-the-art

Modern theoretical spectroscopy allows for the description and the determination of energy levels of medium-sized molecular systems and of an ensemble of these species, either strongly or weakly bound, close to their ground state vibrational level. The applied methodologies depend on the size and on the accuracy needed. Nevertheless, the accuracy of such methods deteriorates as the level of rovibrational excitation increases (at least close to dissociation), with the floppiness of the molecular system, or when the potential energy surface anharmonicities, vibrational mode couplings and dipole anharmonicities become strong. For electronic excited states, additional complications arise in the vicinity of potential energy surfaces artefacts, such as conical intersections, avoided crossings, degeneracy (e.g. at linearity for Renner-Teller systems). State-of-the-art experimental studies show that it is mandatory to consider these effects for the assignment and the interpretation of the spectra of these species and for the understanding and the control of their reactivity. New methodologies are needed. This workshop will be helpful in this respect.

## Objectives

The aim of this preparatory meeting is to gather the scientific organization committee and the local organising committee in order to:

- complete the list of the invited speakers
- discuss additional financial support requests and sponsoring
- discuss material organisation (housing, travel, ...)

- discuss social program
- Website

## Participant List

This list corresponds to the scientific organizing committee (SOC) of the conference:

- Chair: M. Hochlaf\* (U. Paris-Est, France. Email: [hochlaf@univ-mlv.fr](mailto:hochlaf@univ-mlv.fr))
- Co-chair: D. Lauvergnat\* (U. Paris-Sud, France. Email: [David.Lauvergnat@u-psud.fr](mailto:David.Lauvergnat@u-psud.fr))
- Co-chair : R. Linguerri (U. Marne-la-Vallée, France. Email: [Roberto.Linguerri@univ-mlv.fr](mailto:Roberto.Linguerri@univ-mlv.fr))
- G. Chambaud\* (U. Paris-Est, France. Email: [chambaud@univ-mlv.fr](mailto:chambaud@univ-mlv.fr))
- G. Császár\* (Eötvös University, Hungary. Email: [csaszar@chem.elte.hu](mailto:csaszar@chem.elte.hu))
- C. Leforestier\* (U. Montpellier 2, France. Email: [Claude.Leforestier@univ-montp2.fr](mailto:Claude.Leforestier@univ-montp2.fr))
- J. Lievin (U. Libre de Bruxelles, Belgium. Email: [jlievin@ulb.ac.be](mailto:jlievin@ulb.ac.be))
- C. Pouchan\* (UPPA, France. Email: [claude.pouchan@univ-pau.fr](mailto:claude.pouchan@univ-pau.fr))
- M. L. Senent\* (CSIC, Spain. Email: [senent@iem.cfmac.csic.es](mailto:senent@iem.cfmac.csic.es))
- V. Spirko (Academy of Sciences, Czech Republic. Email: [vladimir.spirko@jh-inst.cas.cz](mailto:vladimir.spirko@jh-inst.cas.cz))

\* agreed already.