



US-Africa Initiative Workshop

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Research Orientation:

Molecular Quantum Dynamics

The main interest of our group is to use and develop quantum dynamical methods to describe accurately phenomena in the gas and condensed phase with applications in astrophysics, atmospheric chemistry, combustion, catalysis.

- Our group focuses on wave functions approach to describe the nuclear dynamics: specifically we are using the [MultiConfiguration Time Dependent Hartree \(MCTDH\) method](#) in our research.
- We are involved in various collaborations with groups in the US (Missouri S&T), France (CNRS, Univ. Paris-Saclay, Univ. Montpellier), Germany (Univ. Heidelberg) and Switzerland (EPFL).
- We are open to discussion on potential applications of wave function based methods in Condensed Matter Physics.
- Recently funded research is shown [here](#).



Herve Tajouo Tela

PhD student at ICTP-EAIFR,
Working on the spectroscopy and
dynamics of small water clusters.

Research Directions and Possible Collaborations

- In our group we have expertise in the determination of **vibrational signatures, infrared and UV absorption spectra** of molecular systems of reasonable sizes: in the recent years we studied ozone, nitrogen dioxide, Criegee intermediates and water clusters.
- A recent topic of interest in our group is the study of **photocatalytic processes** using wave function based approach: we intend to try a different approach to gain additional insights on these processes with the aim of designing better catalysts.
- Our group has a strong interest in **method development**: in particular we are working on means to extend wave function based quantum dynamical approach to study condensed phase systems accurately.
- A short exhibit of recent work is available [here](#).