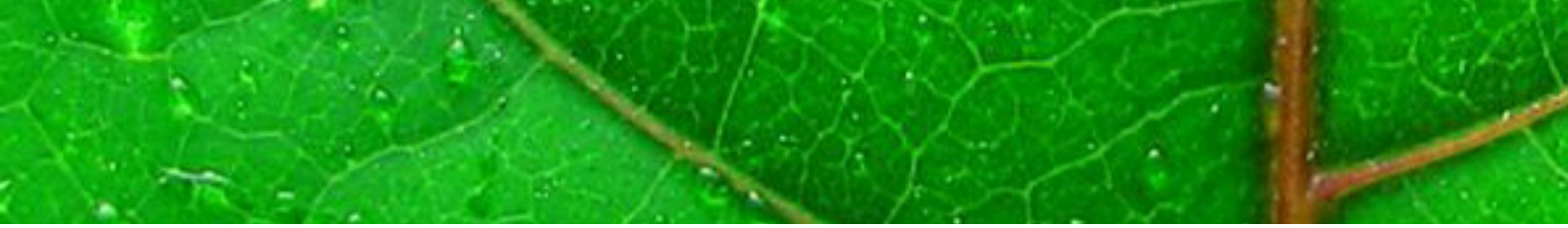


CAPT

Analytical, Physical and Theoretical Chemistry

Scientific skills

Quantum Chemistry, Molecular Dynamics and Scientific Computing

Chemical reactivity

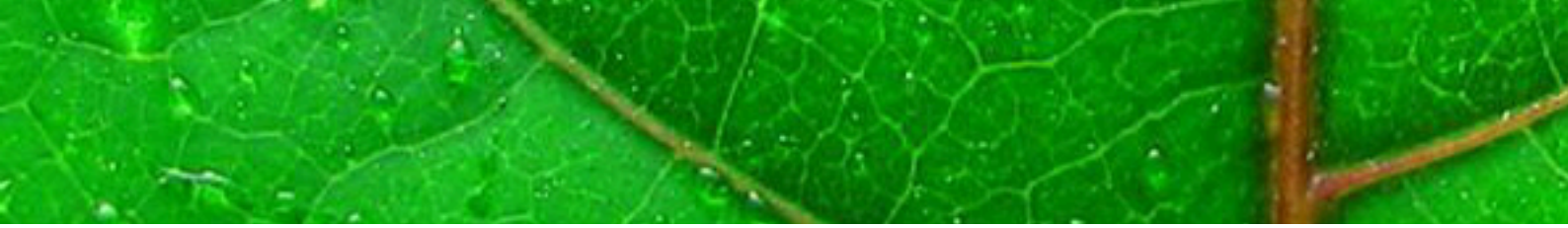
Characterization of short-lived chemical species

Isotopy - Speciation

Spectroscopy / coupled spectrometry

Separative strategies - 2D / 3D chemical imaging

Electrochemistry - Metrology



Research areas

Development of algorithms and computational strategies

- Contribution to the CRYSTAL Code:
- A program for the ab inition investigation of crystalline solids
- New algorithms to compute the anharmonic vibrational spectra
- IR identification of dominant molecular motifs : discerning intermolecular association phenomena
- Quantum chemical design of graphene-based systems for non-linear optical applications
- Surface reactivity of electrode materials
- Understanding of the electronic properties involved by first principles calculations

Trace and ultratrace metal speciation analysis

- Need of a high sensitivity: attogram (10^{-18}) with molecular resolution

Micro – and ultratrace analysis with high precision isotopic resolution

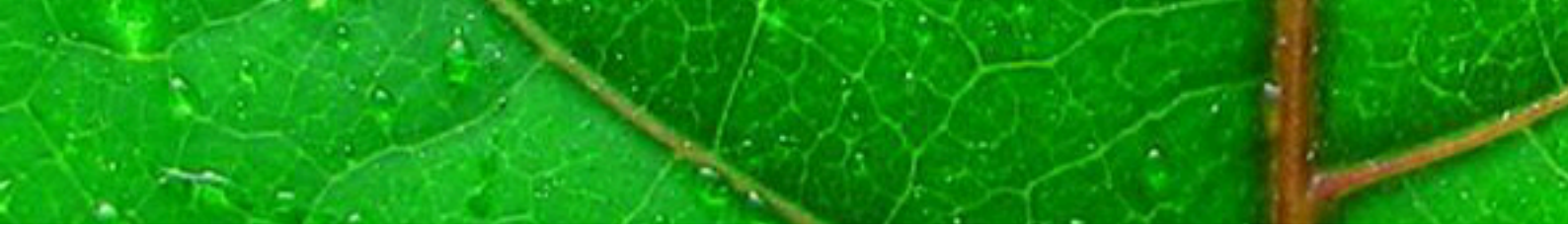
- ***Challenge***: How to measure precisely the isotope ratios using short transient signals?
- ***Developments***: New instrumental couplings, New computational algorighms, Correction of the isotopic drift by synchronisation of detectors

Complex Matrices

- Development of original methodologies for characterization and molecular dynamics of complex systems: C2MC

Molecular architectures: mechanisms and properties

- Reactivity of molecular systems (molecular orbital energies in the valence region) by combined experimental (UV Photoelectron Spectroscopy) and theoretical approach (quantum calculations)
- Understanding and tuning properties of molecules for various applications, catalyst design



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Publications