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Université Claude Bernard Lyon 1

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Research proposal for "contrats doctoraux 2024"
Ecole Doctorale Chimie, Université Claude Bernard Lyon1

Investigating Oxidative Transformations at the Soil-Atmosphere Interface: Bridging ROS and RNS Cycles

Étude des Mécanismes d'Oxydation à l'Interface Sol-Atmosphère : Établissement des Liens entre les Cycles des ROS et RNS

Keywords: Reactive Species, Soil-Atmosphere Interface, Nitrogen Oxides, Kinetics, Laboratory Experiments

Scientific context. In the presence of oxygen, the lifetime of chemical species is primarily linked to oxidation processes. Those limit the accumulation of compounds in the environment, thereby reducing their environmental, health, and social impact.

Specifically, at the soil-atmosphere interface (soil surface), such mechanisms are initiated by the presence of reactive oxygen species (ROS; ROS ≡ $^{\bullet}OH$, H_2O_2, $HO_2^{\bullet}/O_2^{-\bullet}$, $RO_2^{\bullet}$). ROS are formed through processes derived from the photolysis of nitrates/nitrites, organic matter, or chemical reactions involving redox activities such as (photo-)Fenton reactions in the presence of transition metals. However, it is becoming increasingly evident that reactive nitrogen species (RNS; RNS ≡ NO, HNO, NO_2, $HONO/NO_2^-$, $ONOOH/ONOO^-$, $OONOOH/OONOO^-$) are important mediators of ROS concentration at the soil-atmosphere interface. Furthermore, NO, NO_2 and HONO are volatile species that can be emitted from soils to the atmosphere, where they play a critical role in maintaining the oxidizing capacity of the atmosphere and the formation of secondary products such as tropospheric ozone or secondary aerosols. While chemical models exist for aquatic and atmospheric environments allowing us to assess their impact, nothing comparable exists for soils. To address this, *it is necessary to develop fundamental knowledge about the mechanisms and reaction kinetics that facilitate oxidative transformations at the soil-atmosphere interface*.

Missions. The objective of this project is to develop a scientific framework for understanding the chemical mechanisms that control the fate of species at the soil-atmosphere interface. The central hypothesis of the project is that the fate of species depends on 1) the chemical processes that control ROS formation, and 2) that the RNS chemistry plays a major role.

The position includes tasks on analytical development and research in chemical kinetics and mechanistic studies. The selected candidate will be responsible for developing experimental protocols for laboratory studies on the (photo-)generation and transformation of ROS and RNS on the surface of real soil samples or using organic and mineral material as proxies. For this purpose, he/she may use reactors and will have access to instruments based on various analytical techniques such as high-resolution mass spectrometry, chemiluminescence, fluorescence and, UV-Vis absorption.

Profile of the candidate: We are looking for a talented and motivated PhD student, with a background in physical chemistry, environmental chemistry, or analytical chemistry. The PhD candidate should hold a MSc degree (or equivalent). Interested candidates are encouraged to send their resumes.

Team: Be part of the CARE research team! We believe in teamwork and inclusivity. We want to create a welcoming environment, offering an exciting opportunity for PhD students to contribute to cutting-edge global research - IRCELYON

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References:

Additional reading: **10.1021/acs.estlett.0c00806**