

## Programme de la Journée Scientifique 2022

### du Labex CaPPA

Jeudi 10 mars 2022  
Amphithéâtre Pascal  
Cité Scientifique, IMT Nord Europe  
Villeneuve d'Ascq

8:30-9:00	<b>Accueil - Café</b>
9:00-9:25	<b>Introduction</b> – Point d'avancement du projet CaPPA.
9:30-10:45	<b>Synthèse des activités scientifiques 2021</b> (1 <sup>ière</sup> partie) *
9:30-9:55	WP6 : "Box modelling of the atmospheric chlorine chemistry", <i>Zainab Srour</i>
9:55-10:20	WP5 : "Impact of fuel composition on primary and secondary aeronautic emissions: gaseous and particulate chemical characterization at molecular level", <i>Raphael Barrellon-Vernay</i>
10:20-10:45	WP4 : "Improved characterization of volcanic SO <sub>2</sub> emissions and plume dispersion using inverse modelling assimilating TROPOMI, OMPS and IASI observations into an Eulerian chemistry-transport model", <i>Abhinna K. Behera</i>
10:45-11:00	<b>Pause</b>
11:00-11:30	<b>Poster flash</b> (liste en page 3)
11:30-12:15	<b>Session Poster</b>
12:15-13:00	<b>Buffet</b>
13:00-13:45	<b>Café - Posters</b>
13:45-15:00	<b>Synthèse des activités scientifiques 2021</b> (2 <sup>ième</sup> partie) *
13:45-14:10	WP1 : "Nighttime atmospheric degradation of biomass burning compounds: the fate of methylated furan compounds", <i>Fatima Al Ali</i>
14:10-14:35	WP2 : "Synergic retrieval of atmospheric properties using visible and thermal infrared spectrum", <i>Marcos Herreras-Giralda</i>
14:35-15:00	WP3 : "Aerosol optical and chemical properties at the ATOLL site", <i>Alejandra Velazquez-Garcia</i>
15:15-16:00	<b>Conférence Plénière</b> (visio) – Andreas Zuend, Mac Gill University « Modeling of aerosol hygroscopicity, phase separation and cloud droplet activation » ** <a href="https://univ-lille-fr.zoom.us/j/92147275016?pwd=N29pbzB1ODFWYUhhBRkFFZFJzbjNwQT09">https://univ-lille-fr.zoom.us/j/92147275016?pwd=N29pbzB1ODFWYUhhBRkFFZFJzbjNwQT09</a>
16:00-16:30	<b>Posters - Café</b>
16:30	<b>Clôture de la journée</b>

\* Découpage par WP : bilan 2021 par les WPs leaders (5'), présentation scientifique (15'), questions (5')

\*\* Résumé en page 2 de ce programme



## Online seminar at Labex CaPPA scientific day

**Andreas Zuend, Mac Gill University**

March 10, 2022 – 15:15 - 16:00

<https://univ-lille-fr.zoom.us/j/92147275016?pwd=N29pbzB1ODFWYUhBRkFFZFJzbiNwQT09>

**Title:**

Modeling of aerosol hygroscopicity, phase separation and cloud droplet activation

**Abstract:**

The water uptake characteristic (hygroscopicity) of atmospheric aerosols is among several key properties controlled by chemical composition. The hygroscopicity is relevant for particle size, cloud droplet activation, and interactions with radiation. The equilibrium state of a particle is affected by nonideal thermodynamic mixing within its condensed phases and the simultaneous partitioning of semivolatile organic and inorganic species. The occurrence of liquid–liquid phase separation in mixed organic–inorganic particles can affect the aerosol mass concentration, phase viscosities, and particle surface properties. Thermodynamic and dynamic models of these processes attempt to provide predictions for use in detailed single-particle models as well as large-scale atmospheric models. However, a trade-off exists between the level of affordable chemical complexity, available information, and computational costs. In this seminar, we will introduce a relatively detailed framework based on the AIOMFAC model as well as a reduced-complexity organic aerosol model, which offers the ability to process input information typically available in large-scale air quality models and/or data from field studies. We will discuss applications of these models toward a predictive understanding of aerosol hygroscopicity, gas–particle partitioning, and cloud droplet activation.

## Liste des posters:

- P1 : "Synergy of Mie-Raman-fluorescence lidar and Radiometer measurements for aerosol hygroscopicity studies"  
Robin Miri
- P2 : "Biowaste volatile organic compounds emissions and potential for particle formation"  
Kwathar M. Haider
- P3 : "Millimeter-wave spectroscopy of methylfuran isomers: local vs global treatment of the internal rotation".  
Jonas Bruckhuisen
- P4 : "Cavity-enhanced Faraday rotation measurement for OH monitoring"  
Minh Nhut Ngo
- P5 : "Differentiating indoor and outdoor individual exposure to particles: methodology and first results"  
Jérôme Chesneau
- P6 : "Mixing State of Atmospheric Particles during Pollution Events in an Urban and Industrialized Area"  
Soulemene Ngagine
- P7 : "Predictive simulations of core electron binding energies of halogenated species interacting with solvent environment from relativistic quantum embedding calculations"  
Richard O. Opoku
- P8 : "Assessing MP2 frozen natural orbitals in relativistic correlated electronic structure calculation"  
Xiang Yuan
- P9 : "Absolute absorption cross section of the C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> radical and kinetic of its self-reaction : Rate constant and branching ratio "  
Cuihong Zhang
- P10 : "OH-initiated atmospheric degradation of 2,3,4,5-chlorophenol insecticide"  
Hisham K. Al Rawas
- P11 : "OH-initiated atmospheric degradation of phosmet insecticide"  
Reem Al Mawla
- P12 : "Reactivity of OH with CH<sub>3</sub>I in the presence of H<sub>2</sub>O"  
Sonia Taamalli
- P13 : "Reactivity of H atoms with halogenated polycyclic aromatics hydrocarbons"  
Nesrine Bekkal
- P14 : "Kinetic study of heterogeneous reactions on oleic acid clusters using a QM/MM approach  
Akilan Rajaman
- P15 : "Unexpected phase behavior of complex particles containing ammonium sulfate, glycolic acid and oligomer:  
Study at the single particle scale"  
Mikel Sader
- P16 : « Polluen » : le pollen à l'ère de l'anthropocène  
Marie Choël