Title: Modelling of ice formation at low temperature from an atmosphere containing water vapour and VOCs with or without contact with a mineral surface.

Place: Laboratoire Interdisciplinaire Carnot de Bourgogne, Dijon
Financial support: DECOLAIR project supported by l'Ecole Universitaire de Recherche EIPHI, by the Région Bourgogne Franche-Comté and by FEDER. 12 months, gross salary – around 2500 €/month.

Context: This post-doctoral project is part of a research program dedicated to the selective trapping of atmospheric volatile organic compounds (VOCs) in the presence of water vapour at low temperature on solid water in presence of mineral surfaces. This is a theoretical study using molecular simulation methods (Monte-Carlo and Molecular Dynamics) that will be conducted in addition to experimental studies conducted in parallel. The work will focus on ice germination and growth in water vapour atmospheres containing VOCs. The aim will be to determine how VOCs can stabilize the formation of one type of ice rather than another, but also accelerate or slow down their formation. This work therefore aims to gain a better understanding of the type, shape and size of ice formed for a given duration and under given atmospheric conditions and its consequences on the trapping of VOCs.
It is known experimentally that certain mineral surfaces favour the formation of ice (in its different forms) or on the contrary inhibit their formation. The mechanisms causing these effects are poorly known and are very important for understanding the trapping of atmospheres on ice (knowledge of these mechanisms will also help to optimize the design of low temperature sensors). An important aspect of this work will therefore be to study the effect of the presence of mineral surfaces (hydrophobic or hydrophilic) on ice formation and VOC trapping.
The program is subdivided into two main tasks:
(1) - Determination of VOC adsorption isotherms on (ideal) ice models by molecular simulations
(2) - Modelling of ice germination and growth at low temperature from an atmosphere containing water vapour and VOCs with or without contact with a mineral surface.
One of the direct applications of this study, which will be the theoretical counterpart of the experimental research of the DECOLAIR project, is the use of adsorbents and gas sensors to purify air at temperatures below 0°C where water solidifies. The project will be done in collaboration with the institute UTINAM (Sylvain Picaud) at the University of Besançon for astrophysical implications of selective adsorption of COVs on ice.

Goals:
- Thermodynamic and dynamic models of ice germination and growth from an atmosphere containing water vapour and VOCs with or without a mineral surface at low temperature (below 0°C).
- Model of selective trapping of VOC molecules within or in contact with ice and comparison with experimental results from experiments carried out in the laboratory as part of the DECOLAIR project.

Candidate profile: PhD in physical chemistry/physics. Knowledge in classical molecular simulation, adsorption, germination/growth of crystal.
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