Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.16798

Molecular-scale studies of organic aerosols : from the formation of aerosol precursors to the characterization of the aerosol interactions with surrounding water molecules.

BASTIEN RADOLA, DELPHINE VARDANEGA-BONNETON AND **SYLVAIN PICAUD**

Institut UTINAM - UMR 6213 CNRS/UBFC

Presenting Author: sylvain.picaud@univ-fcomte.fr

Atmospheric aerosols play a central role on current atmospheric research, because aerosol particles have a direct effect on climate not only by scattering and absorbing solar radiation but also by scattering, absorbing, and emitting thermal radiation. They also have an indirect effect by acting as condensation nuclei for water, thus impacting on cloudiness. Organic matter represents an important fraction of the fine aerosol mass with relative abundance depending on, e.g., location, time, and meteorological conditions.

Given the complexity of aerosol chemistry, modeling studies based on numerical simulations at the molecular level is an important way to get insights on the corresponding systems, complementary to numerous observations and laboratory characterizations.

In our group, we use various theoretical methods to achieve a better characterization of the aerosol behavior, at the molecular scale.

Thus, DFT calculations have been devoted to model the formation of aerosol precursors via, e.g., the interactions between a small number of sulfuric acid and small organic molecules [1,2]. In addition, classical molecular dynamics simulations considering much larger systems (i.e., made of hundreds of organic molecules) have been undertaken to model the evolution with temperature of organic aerosol nanoparticles interacting with different amounts of water molecules [3-5].

Bibliography

[1] Radola, B., Picaud, S., Ortega, I.K. (2022) DFT study of the formation of atmospheric aerosol precursors from the interaction between sulfuric acid and benzenedicarboxylic acid molecules. J. Phys. Chem. A **126**, 1211-1220.

[2] Radola, B., Picaud, S., Ortega, I.K., Ciuraru, R. (2021). Formation of atmospheric molecular clusters from organic waste products and sulfuric acid molecules. A DFT study. Environ. Sci. : Atmos. **1**, 267-275.

[3] Radola, B., Picaud, S., Vardanega, D., Jedlovszky, P. (2017). Analysis of Mixed Formic and Acetic Acid Aggregates Interacting with Water. A Molecular Dynamics Simulation Study. J. Phys. Chem. C **121**, 13863-13875.

[4] Radola, B., Picaud, S., Vardanega, D., Jedlovszky, P. (2015). Molecular Dynamics Simulations of the Interaction between Water Molecules and Aggregates of Acetic or Propionic Acid Molecules. J. Phys. Chem. B **119**, 15662-15674.

[5] Vardanega, D., Picaud, S. (2014). Water and formic acid aggregates: A molecular dynamics study. J. Chem. Phys. **141**, 104701 :1-8.