Université de Lille

Area Cross Disciplinary Project Lille

Aerosol at the heaRt of the Earth/Atmosphere system

Master 2 - Research Training – 01/02 to 30/06/2026

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AREA Work Package: (1, 2 or 3) 2

Molecular insights on the surface propensity of organosulfates

Organosulfates (OS) are sulfur-containing compounds that play an important role in atmospheric composition. For example, methyltetrol sulfates (MTS), which are derived from the photochemical oxidation of isoprene in low-nitric oxide environments, are prominent atmospheric OS, particularly in heavily forested regions where isoprene emissions—affected by anthropogenic pollutants—are significant.

Despite a good understanding of OS formation pathways, uncertainties remain regarding their kinetics and transformation routes in the atmosphere. In particular, there is a need to characterize the surface behavior of OS at the air/water interface, as this property can impact their surface availability for heterogeneous chemistry. Classical molecular dynamics simulations can help characterize this behavior, particularly by calculating surface tensions, which are important observables in atmospheric chemistry and will be measured by the experimental team in Hong Kong. Modeling concentrated organosulfate solutions requires explicitly accounting for possible polarization effects induced by uncompensated charges.

The objective of the internship is to conduct classical molecular dynamics simulations and eventually ab initio MD simulations to characterize the surface behavior of selected organosulfates and eventually mixtures.

Key words: MD simulations, surface tension, surface propensity