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

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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

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