Computational investigation of multiphase chemical mechanisms in atmospheric aerosols and water droplets

Rawan AbouHaidar[2], Sana Bougueroua[2], Denis Duflot[1], Marie-Pierre Gaigeot[2], Barbara Wyslouzil[3], Céline Toubin[1]

[1] Univ. Lille, CNRS, UMR 8523 – PhLAM – Physique des Lasers Atomes et Molécules, F-59000 Lille, France.

[2] Université Paris-Saclay, University Evry, CY Cergy Paris Université, CNRS, LAMBE UMR8587, 91025 Evry-Courcouronnes, France

[3]The Ohio State University - William G. Lowrie Department of Chemical and Biomolecular Engineering, Columbus, OH 43210-1226, USA.

Gas–liquid and air–liquid interfaces play a central role in atmospheric chemistry by controlling reaction kinetics, phase partitioning, and chemical transformations. Gaining molecular-level insight into these interfacial processes is essential for predicting atmospheric behavior and its implications for climate and the environment. Molecular dynamics (MD) and quantum mechanical (QM) approaches provide complementary perspectives on the multiphase chemistry and mechanisms of freezing.

This talk highlights applications of these molecular-level methods. MD simulations elucidate interfacial organization and partitioning between surface and bulk phases, which strongly influence uptake processes, surface properties, and ice nucleation. In particular, graph theory analysis has revealed how short-chain alcohols modify the hydrogen-bonding network of interfacial water, offering new perspectives on the early stages of freezing relevant to climate science. In parallel, QM and hybrid QM/QM' methods captured heterogeneous reactivity, including explicit solvent effects, and predict heterogeneous rate constants that may differ by several orders of magnitude from gas-phase reactions.

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References

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