EGU21-8258, updated on 05 Dec 2022
https://doi.org/10.5194/egusphere-egu21-8258
EGU General Assembly 2021

On the interface of organic aerosols: molecular level understanding of surface melting, mixing and water adsorption/desorption dynamics

Josip Lovrić, Xiangrui Kong, Sofia M. Johansson, Erik S. Thomson, and Jan B. C. Pettersson
Department of Chemistry and Molecular Biology, Atmospheric Science, University of Gothenburg, SE-412 96 Gothenburg, Sweden

The detailed description of organic aerosols surfaces in the atmosphere remains an open issue, which limits our ability to understand and predict environmental change. Important research questions concern the hydrophobic/hydrophilic character of fresh and aged aerosols and the related influence on water uptake in solid, liquid as well in intermediate state. Also, surface characterization remains big challenge but we find it reachable by conjunction of Molecular Dynamics (MD) simulations and the environmental molecular beam (EMB) experimental method. A picture of the detailed molecular-level behavior of water molecules on organic surfaces is beginning to rise based on detailed experimental and theoretical studies; one example is a recent study that investigates water interactions with solid and liquid n-butanol near the melting point [1], another example focus on interaction of water with solid nopinone [2]. From the other side, in order to characterize surface properties during and before melting we employ MD simulations of n-butanol, nopinone and valeric acid. Nopinone ($C_9H_{14}O$) is a reaction product formed during oxidation of β-pinene and has been found in both the gas and particle phases of atmospheric aerosol. n-butanol (C_4H_9OH) is primary alcohol, naturally occurs scarcely and here serves as good representative for alcohols. In the same way valeric acid ($CH_3(CH_2)_3COOH$) serves as a good representative for a family of carboxylic acids. Valeric acid is, as n-butanol, straight-chain molecule. We show that a classical force field for organic material is able to model crystal and liquid structures. The surface properties near the melting point of the condensed phase are reported, and the hydrophobic and hydrophilic character of the surface layer is discussed. Overall surface melting dynamic is presented and quantified in the terms of structural and geometrical properties. Mixing of a methanol with the solid nopinone surface is examined and hereby presented.

References

[1] Johansson, S. M., Lovrić, J., Kong, X., Thomson, E. S., Papagiannakopoulos, P., Briquez, S., Toubin, C, Pettersson, J. B. C. (2019). Understanding water interactions with organic surfaces: environmental molecular beam and molecular dynamics studies of the water–butanol system. Physical Chemistry Chemical Physics. https://doi.org/10.1039/C8CP04151B

[2] Johansson, S. M., Lovrić, J., Kong, X., Thomson, E. S., Hallquist, M., & Pettersson, J. B. C. (2020).

Experimental and Computational Study of Molecular Water Interactions with Condensed Nopinone Surfaces Under Atmospherically Relevant Conditions. The Journal of Physical Chemistry A, acs.jpca.9b10970. https://doi.org/10.1021/acs.jpca.9b10970

Keywords: Molecular Dynamics, organic crystal, organic aerosols, water uptake, surface procesess, molecular level