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Trapping on organic surfaces: a molecular level perspective

Abstract (no more than 2000 characters)

Aerosols and clouds are of central importance for climate on Earth due to their effects on the chemistry and radiation budget of the atmosphere. Organic compounds are of particular interest due to their abundance and their intricate changes during slow oxidation in the atmosphere, which result in formation of secondary organic aerosols and coatings on existing particles.
In particular, organic coating is known to significantly alter the surface physicochemical properties of soot particles. However, the specific properties on the coating are difficult to predict because the molecular arrangement of the layer is profoundly influenced by the interactions between organics and soot surface.
We propose to study by means of classical molecular dynamics simulations the effect of an organic coating (nopinone) on a graphite surface on the trapping of organic molecules (butanol or formic acid). The graphite is analogous to highly ordered type of soot particles in the atmosphere, and the thin nopinone coating can be regarded as a model organic coating on aged soot. The nopinone multilayer is a model organic aerosol on its own.
The results of the simulations will be compared to molecular beam experiments performed in Goteborg [Kong et al].

Key words: uptake, adsorption, trapping, organic coating, soot, molecular dynamics