**PhD thesis title:**

# Engineered Nanoparticles in the Environment: Sorption Behavior of Carbon Nanotubes in Aquatic Systems

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## Abstract

With the fast development of nanotechnology, the production of engineered nanoparticles (ENPs) increases rapidly. ENPs will inevitably be released into the environment and may become important emerging pollutants. Interactions between organic contaminants and ENPs can alter the environmental fate of both materials (e.g., ENP-bound cotransport of contaminants). Carbon nanotubes (CNTs) are one type of widely produced ENPs. CNTs have a very strong affinity toward organic contaminants and have been proposed as superior sorbents for environmental remediation as well as for analytical applications. Understanding the interactions between organic contaminants and CNTs is therefore essential for evaluating the materials' potential environmental impact as well as the potential efficiency as superior sorbent.

The objective of this PhD thesis is to advance the understanding of interactions between CNTs and organic compounds, polycyclic aromatic hydrocarbons (PAHs) in particular. The sorption behavior of CNTs was investigated over a range of conditions that have never been investigated before, using a suitable alternative to the classical sorption experimental set up (i.e., passive sampling method). Sorption data were combined to extensive CNTs characterization and data analysis to better understand sorption behavior in the low concentration range, for very hydrophobic compounds and in conditions where CNTs are dispersed. The main findings can be summarized below:

- Conversely to previous studies carried out at unrealistic high concentration ranges, sorption isotherms in the low concentration range (pg–ng/L) indicate that sorption can be described using single sorption coefficients.

- Sorption coefficients for 13 PAHs (11 of which have never been reported before) showed that no competition occurred in the low concentration range and sorption affinity was directly related to the solubility of the subcooled liquid of the compounds.
- Conversely to previous observations restricted to large aggregates, our study highlights the importance of considering both the size and structure of sorbent aggregates.
- To date, limited published data generally suggested that the presence of functional groups on the CNTs decrease the sorption of nonpolar compounds. We here analyzed differences due to the nature of the functionalization and demonstrated that the impact on sorption behavior greatly depends on the CNT dispersion status. The suppression of sorption by natural dispersants greatly depends on the CNTs surface chemistry.
- Aggregation/dispersion significantly affects the sorption behavior of CNTs. Both the nature (e.g., sonication, presence of dispersants or functionalization) and the chronological sequence of the dispersion events are essential in determining the extent and irreversibility of the effects on sorption behavior of CNTs.

Our results show that a number of factors that were not thoroughly considered to date are essential when evaluating the interactions between organic contaminants and carbonaceous nano-sorbents. The sorption behavior of ENPs is a complex process, especially when accounting for colloidal behavior, and many research questions remain unanswered. The use of more suitable and robust methods, such as that develop in the present work, opens up a way to study sorption for a wider range of compounds and ENPs, and over a wide range of relevant conditions. The data generated will be vital for evaluating the materials' potential environmental impact as well as the potential future applications.