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# The role of the bile salt surfactant sodium deoxycholate in aqueous two-phase separation of single-wall carbon nanotubes revealed by systematic parameter variations



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## ABSTRACT

Aqueous two-phase (ATP) extraction has been demonstrated as a fast, scalable, and effective separation technique to sort single-wall carbon nanotubes (SWCNTs) according to their diameter and chiral structure. The exact mechanism behind the chirality-dependent migration of SWCNTs between the two phases is however not completely understood, and depends on many parameters (e.g., choice of surfactants and their concentration, pH, temperature, ...), making it difficult to optimize the multivariable parameter space. In this work, we present a systematic study of the choice and concentration of specific surfactants on the ATP sorting, by performing a series of single-step ATP separations in which each time only one parameter is systematically varied, while monitoring the structure-specific migration of every SWCNT chirality between both phases with detailed wavelength-dependent spectroscopy. These systematic studies reveal that the diameter-dependent stacking of a discrete number of sodium deoxycholate molecules fitting around the SWCNT circumference determines the separation order in the form of a periodically modulated pattern as a function of SWCNT diameter. Addition of cosurfactants can be used to compete with the bile salt surfactant to enhance the separation yields, but does not affect the sorting order. The results are afterwards directly applied to predict the parameters required to separate specific chiral structures in just two ATP steps.

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## 1. Introduction

Since their discovery in 1993 [1] the interest in single-wall carbon nanotubes (SWCNTs) has grown exponentially. Their well-defined structure-dependent electronic and optical properties [2] combined with unique mechanical and thermal properties, make SWCNTs fascinating materials for an extensive set of applications in nanoelectronics, photonics, photovoltaics and biochemical sensing [3]. However, a longstanding issue for their implementation in actual devices remains that synthesis methods invariably produce mixtures of different diameters, chiral structures, and metallic and semiconducting tubes, each with their specific electronic and

optical properties. While significant progress is being made to synthesize extremely narrow diameter distributions [4–8], most synthesis methods are not yet sufficiently selective and versatile to produce any chirality on demand, and thus an appropriate versatile, scalable, cheap and fast separation technique is crucial to create an industrial breakthrough. A variety of separation techniques have been introduced in the field and were recently reviewed in Refs. [8,9], such as dielectrophoresis [10], density gradient ultracentrifugation (DGU) [11,12], selective polymer wrapping [13–15], DNA- [16,17] or surfactant- [18,19] solubilization followed by size-exclusion chromatography and more recently aqueous two-phase extraction (ATP) [20]. ATP in particular shows promise to become a fast, highly scalable and easily tunable separation method. This technique, developed in the 1980s for biochemical separations [21–23], has more recently been successfully applied to separate SWCNTs [24–38]. In ATP, two water-soluble, yet immiscible polymers (e.g., polyethylene glycol [PEG] and dextran) are mixed together at sufficiently high concentration, after which they

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