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Molecular Dynamics of Adsorption: Interaction between Benzoic Acid in Solution and Functionalized Carbon Nanotubes[1] ISKINDER ARSANO, Akron Univ, KEVIN FEEZEL, St.Vincent-St.Mary High School, Akron, OH, XINGMAO MA , Texas AM University, SAIKAT TALAPATRA , Southern Illinois University at Carbondale, MESFIN TSIGE, Akron Univ — Adsorption of organic contaminants is among the promising applications of carbon nanotubes that have provoked academic and industrial interest. The current work investigates, through molecular dynamics simulations, filtration of benzoic acid-contaminated water by use of single-walled carbon nanotubes. Such a study inevitably resides at the frontier between molecular and environmental research. Extensive theoretical and experimental studies have shown that adsorption on nanotubes is characterized by the presence of large specific surface areas and the availability of different adsorption sites on the nanotubes. In keeping with this understanding we have carboxylated the carbon nanotubes at different percentages relative to the number of the nanotube carbons. The variability of hydrogen bonding, as a function of radial distance from nanotube, between the different hydrogen containing species in our system is reported. Benchmark values of tube length, tube radius, and concentration of benzoic acid in water were used to examine adsorption properties. The observations were further extended to make recommendations on the scalability of nanotube filtration to input values not explored in the present work.

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