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Potential of Mean Force between Aqueous Single Walled Carbon Nanotubes in Surfactant Solutions[1] ALBERTO STRIOLO, The University of Oklahoma, NAGA RAJESH TUMMALA, BRIAN H. MORROW, OU MOLECULAR SCIENCE AND ENGINEERING TEAM — Molecular dynamic simulations were conducted to calculate the effective potential of mean force (PMF) between two (6,6) SWNTs in the presence of aqueous surfactants at room conditions. The surfactants considered include sodium dodecyl sulfate (SDS) and flavin mononucleotide (FMN) surfactants. In the absence of surfactants our results show, as expected, a strongly attractive SWNT-SWNT PMF at short nanotube-nanotube separations. The presence of surfactants modulates the PMF profile. In the case of SDS we found that the potential of mean force does not depend significantly on the SDS surface density. The PMF shows a long-ranged weak repulsion between the SWNTs in the presence of the surfactants, coupled to strong attractive and repulsive regions when the SWNTs are close to each other. Unfortunately, the repulsive peak is not strong enough to prevent the aggregation of carbon nanotubes. Because FMN surfactants contain an aromatic isoalloxazine moiety and a chiral phosphate group, they couple more tightly with the SWNTs and yield a pronounced repulsive force between approaching SWNTs. Our results will help us identify the surfactant properties that allow us to manipulate nanotube-nanotube effective interactions. This is the key for designing nanotube-specific dispersing agents.

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Alberto Striolo
The University of Oklahoma

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