REFERENCES

Amama, P. B., Lan, C., Cola, B. A., Xu, X., Reifenberger, R. G., and Fisher, T. S. (2008). Electrical and thermal interface conductance of carbon nanotubes grown under direct current bias voltage. The Journal of Physical Chemistry C, 112, 19727–19733.

Angelikopoulos, P. and Bock, H. (2009). The differences in surfactant adsorption on carbon nanotubes and their bundles. Langmuir, 26(2), 899–907.

Berendsen, H. J. C., Grigera, J. R., abd Straatsma, T. P. (1987). The missing term in effective pair potentials. The Journal of Physical Chemistry, 91(24), 6269–6271.

Bergin, S. D., Sun, Z., Streich, P., Hamílton, J., and Coleman, J. N. (2009). New solvents for nanotubes: Approaching the dispersibility of surfactants. The Journal of Physical Chemistry C, 114(1), 231–237.

Bhushan, B. (2006). Springer handbook of nanotechnology. Berlin: Springer.

Blanch, A. J., Lenehan, C. E., and Quinton, J. S. (2010). Optimizing surfactant concentrations for dispersion of single-walled carbon nanotubes in aqueous solution. The Journal of Physical Chemistry B, 114(30), 9805–9811.

Cadek, M., Coleman, J. N., Ryan, K. P., Nicolosi, V., Bister, G., Fonseca, A., Nagy, J. B., Szostak, K., Béguin, F., and Blau, W. J. (2004). Reinforcement of polymers with carbon nanotubes: The role of nanotube surface area. Nano Letters, 4 (2), 353–356.

Calvaresi, M., Dallavalle, M., and Zerbetto, F. (2009). Wrapping nanotubes with micelles, hemimicelles, and cylindrical micelles. Small 5(19), 2191–2198.

Cheng, A. and Steele, W. A. (1990). Computer simulation of ammonia on graphite. II. Monolayer melting. The Journal of Chemical Physics, 92(6), 3867–3873.

Clark, M. D., Subramanian, S., and Krishnamoorti, R. (2011). Understanding surfactant aided aqueous dispersion of multi-walled carbon nanotubes. Journal of Colloid And Interface Science, 354(1), 144–151.

Dai, H. (2002). Carbon nanotubes: Synthesis, integration, and properties. Accounts of Chemical Research, 35(12), 1035–1044.

Davis, V. A., Parra-Vasquez, A. N. G., Green, M. J., Rai, P. K., Behabtu, N., Prieto, V., Booker, R. D., Schmidt, J., Kesselman, E., Zhou, W., Fan, H., Adams, W. W., Hauge, R. H., Fischer, J. E., Cohen, Y., Talmon, Y., Smalley, R. E., and Pasquali, M. (2009). True solutions of single-walled carbon nanotubes for assembly into macroscopic materials. Nature Nanotechnology, 4(12), 830–834.

Essmann, U., Perera, L., Berkowitz, M. L., Darden, T., Lee, H., and Pedersen, L. G. (1995). A smooth particle mesh Ewald method. The Journal of Chemical Physics, 103(19), 8577–8593.

Frenkel, D. and Smit, B. (1996). Understanding molecular simulation: From algorithms to applications. Orlando: Academic Press, Inc.

Girifalco, L. A., Hodak, M., and Lee, R. S. (2000). Carbon nanotubes, buckyballs, ropes, and a universal graphitic potential. Physical Review B, 62(19), 13104–13110.

Grossiord, N., van der Schoot, P., Meuldijk, J., and Koning, C. E. (2007). Determination of the surface coverage of exfoliated carbon nanotubes by surfactant molecules in aqueous solution. Langmuir, 23(7), 3646–3653.

Haggenmueller, R., Rahatekar, S. S., Fagan, J. A., Chun, J., Becker, M. L., Naik, R. R., Krauss, T., Carlson, L., Kadla, J. F., Trulove, P. C., Fox, D. F., DeLong, H. C., Fang, Z., Kelley, S. O., and Gilman, J. W. (2008). Comparison of the quality of aqueous dispersions of single wall carbon nanotubes using surfactants and biomolecules. Langmuir, 24(9), 5070–5078.

He, X., Guvench, O., MacKerell, A. D., and Klein, M. L. (2010). Atomistic simulation study of linear alkylbenzene sulfonates at the water/air interface. The Journal of Physical Chemistry B, 114(30), 9787–9794.

Hess, B., Kutzner, C., van der Spoel, and D., Lindahl, E. (2008). GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable molecular simulation. Journal of Chemical Theory and Computation, 4(3), 435–447.

Hoover, W. G. (1985). Canonical dynamics: Equilibrium phase-space distributions. Physical Review A, 31(3), 1695–1697.

Islam, M. F., Rojas, E., Bergey, D. M., Johnson, A. T., and Yodh, A. G. (2003). High weight fraction surfactant solubilization of single-wall carbon nanotubes in water. Nano Letters, 3(2), 269–273.

Jang, S. S., Lin, S.-T., Maiti, P. K., Blanco, M., Goddard, W. A., Shuler, P., and Tang, Y. (2004). Molecular dynamics study of a surfactant-mediated decane-water interface: Effect of molecular architecture of alkyl benzene sulfonate. The Journal of Physical Chemistry B, 108(32), 12130–12140.

Lahiri, D., Rouzaud, F., Namin, S., Keshri, A. K., Valdés, J. J., Kos, L., Tsoukias, N., and Agarwal, A. (2009). Carbon nanotube reinforced polylactide-caprolactone copolymer: Mechanical strengthening and interaction with human osteoblasts in Vitro. ACS Applied Materials & Interfaces, 1 (11), 2470–2476.

Lemasson, F. A., Strunk, T., Gerstel, P., Hennrich, F., Lebedkin, S., Barner-Kowollik, C., Wenzel, W., Kappes, M. M., and Mayor, M. (2010). Selective dispersion of single-walled carbon nanotubes with specific chiral indices by poly(N-decyl-2,7-carbazole). Journal of the American Chemical Society, 133(4), 652–655.

Lin, S. and Blankschtein, D. (2010). Role of the bile salt surfactant sodium cholate in enhancing the aqueous dispersion stability of single-walled carbon nanotubes: A molecular dynamics simulation study. The Journal of Physical Chemistry B, 114(47), 15616–15625.

Lu, K. L., Lago, R. M., Chen, Y. K., Green, M. L. H., Harris, P. J. F., and Tsang, S. C. (1996). Mechanical damage of carbon nanotubes by ultrasound. Carbon, 34 (6), 814–816.

Martin, M. G. and Siepmann J. I. (1997). Predicting multicomponent phase equilibria and free energies of transfer for alkanes by molecular simulation. Journal of the American Chemical Society, 119(38), 8921–8924.

Matarredona, O., Rhoads, H., Li, Z., Harwell, J. H., Balzano, L., Resasco, D. E. (2003). Dispersion of single-walled carbon nanotubes in aqueous solutions of the anionic surfactant NaDDBS. The Journal of Physical Chemistry B, 107(48), 13357–13367.

Mayo, S. L., Olafson, B. D., and Goddard, W. A. (1990). DREIDING: A generic force field for molecular simulations. The Journal of Physical Chemistry, 94(26), 8897–8909.

McDonald, T. J., Engtrakul, C., Jones, M., Rumbles, G., and Heben, M. J. (2006). Kinetics of PL quenching during single-walled carbon nanotube rebundling and diameter-dependent surfactant interactions. The Journal of Physical Chemistry B, 110(50), 25339–25346.

Minami, N., Kim, Y., Miyashita, K., Kazaoui, S., and Nalini, B. (2006). Cellulose derivatives as excellent dispersants for single-wall carbon nanotubes as demonstrated by absorption and photoluminescence spectroscopy. Applied Physics Letters, 88(9), 093123–093123.

Myers, D. (2005). The organic chemistry of surfactants. Hoboken: John Wiley & Sons, Inc.

O'Connell, M. J., Boul, P., Ericson, L. M., Huffman, C., Wang, Y., Haroz, E., Kuper, C., Tour, J., Ausman, K. D., and Smalley, R. E. (2001). Reversible water-solubilization of single-walled carbon nanotubes by polymer wrapping. Chemical Physics Letters, 342(3-4), 265–271.

Okazaki, T., Saito, T., Matsuura, K., Ohshima, S., Yumura, M., and Iijima, S. (2005). Photoluminescence mapping of "As-Grown" single-walled carbon

nanotubes: A comparison with micelle-encapsulated nanotube solutions. Nano Letters, 5(12), 2618–2623.

Parra-Vasquez, A. N. G., Behabtu, N., Green, M. J., Pint, C. L., Young, C. C., Schmidt, J., Kesselman, E., Goyal, A., Ajayan, P. M., Cohen, Y., Talmon, Y., Hauge, R. H., and Pasquali, M. (2010). Spontaneous dissolution of ultralong single- and multiwalled carbon nanotubes. ACS Nano 4(7), 3969–3978.

Prakashm, N. (2005). Determination of coefficient of thermal expansion of single-walled carbon nanotubes using molecular dynamics simulations. M.S. Thesis, Department of Mechanical Engineering, The Florida State University, Florida, USA.

Ramesh, S., Ericson, L. M., Davis, V. A., Saini, R. K., Kittrell, C., Pasquali, M., Billups, W. E., Adams, W. W., Hauge, R. H., and Smalley, R. E. (2004). Dissolution of pristine single walled carbon nanotubes in superacids by direct protonation. The Journal of Physical Chemistry B, 108(26), 8794–8798.

Rosen, M. J. (2004). Adsorption of Surface-Active Agents at Interfaces: The Electrical Double Layer. Hoboken: John Wiley & Sons, Inc.

Siepmann, J. I., Karaborni, S., and Smit, B. (1993). Simulating the critical behaviour of complex fluids. Nature, 365(6444), 330–332.

Smit, B., Karaborni, S., and Siepmann, J. I. (1995). Computer simulations of vapor-liquid phase equilibria of n-alkanes. The Journal of Chemical Physics, 102(5), 2126–2140.

Tabakman, S. M., Welsher, K., Hong, G., and Dai, H. (2010). Optical properties of single-walled carbon nanotubes separated in a density gradient: Length, bundling, and aromatic stacking effects. The Journal of Physical Chemistry C, 114 (46), 19569-19575.

Tan, Y. and Resasco, D.E. (2005). Dispersion of single-walled carbon nanotubes of narrow diameter distribution. The Journal of Physical Chemistry B, 109(30), 14454–14460.

Thess, A., Lee, R., Nikolaev, P., Dai, H., Petit, P., Robert, J., Xu, C., Lee, Y. H., Kim, S. G., Rinzler, A. G., Colbert, D. T., Scuseria, G. E., Tománek, D., Fischer, J. E., and Smalley, R. E. (1996). Crystalline ropes of metallic carbon nanotubes. Science, 273 (5274), 483–487.

Tummala, N. R. and Striolo, A. (2009). Curvature effects on the adsorption of aqueous sodium-dodecyl-sulfate surfactants on carbonaceous substrates: Structural features and counterion dynamics. Physical Review E, 80(2), 021408.

Tummala, N. R. and Striolo, A. (2008). Role of counterion condensation in the self-assembly of SDS surfactants at the water-graphite interface. The Journal of Physical Chemistry B, 112(7), 1987–2000.

Tummala, N. R. and Striolo, A. (2009). SDS surfactants on carbon nanotubes: Aggregate morphology. ACS Nano, 3(3), 595–602.

Tummala, N. R., Morrow, B. H., Resasco, D. E., and Striolo, A. (2010). Stabilization of aqueous carbon nanotube dispersions using surfactants: Insights from molecular dynamics simulations. ACS Nano, 4(12), 7193–7204.

Utsumi, S., Kanamaru, M., Honda, H., Kanoh, H., Tanaka, H., Ohkubo, T., Sakai, H., Abe, M., and Kaneko, K. (2007). RBM band shift-evidenced dispersion mechanism of single-wall carbon nanotube bundles with NaDDBS. Journal of Colloid And Interface Science, 308(1), 276–284.

Vaisman, L., Wagner, H. D., and Marom, G. (2006). The role of surfactants in dispersion of carbon nanotubes. Advances in Colloid and Interface Science, 128-130, 37–46.

Wallace, E.J. and Sansom, M.S.P. (2009). Carbon nanotube self-assembly with lipids and detergent: A molecular dynamics study. Nanotechnology, 20, 045101.

Wang, H. (2009). Dispersing carbon nanotubes using surfactants. Current Opinion in Colloid & Interface Science, 14(5), 364–371.

Xu, Z., Yang, X., and Yang, Z. (2010). A molecular simulation probing of structure and interaction for supramolecular sodium dodecyl sulfate/single-wall carbon nanotube assemblies. Nano Letters, 10(3), 985–991.

Yan, L. Y., Poon, Y. F., Chan-Park, M. B., Chen, Y., and Zhang, Q. (2008). Individually dispersing single-walled carbon nanotubes with novel neutral pH water-soluble chitosan derivatives. The Journal of Physical Chemistry C, 112(20), 7579–7587.

Yurekli, K., Mitchell, C. A., and Krishnamoorti, R. (2004). Small-angle neutron scattering from surfactant-assisted aqueous dispersions of carbon nanotubes. Journal of the American Chemical Society, 126(32), 9902–9903.

Zhao, J., Park, H., Han, J., and Lu, J. P. (2004). Electronic properties of carbon nanotubes with covalent sidewall functionalization. The Journal of Physical Chemistry B, 108(14), 4227–4230.

Zheng, M., Jagota, A., Semke, E. D., Diner, B. A., McLean, R. S., Lustig, S. R., Richardson, R. E., and Tassi, N. G. (2003). DNA-assisted dispersion and separation of carbon nanotubes. Nature Materials, 2(5), 338–342.

APPENDICES

Appendix A Calculation of Surface Area of Single-Walled Carbon Nanotubes

The diameter of SWNT is found with:

$$D = \left(\frac{a}{\pi}\right)\left(n^2 + m^2 + nm\right)^{1/2},$$

where D = diameter

a = 0.246 nm

n, m = integers n and m represented by a pair of indices (n,m)

The surface area of SWNT is found with:

$$SA = \pi DL,$$

where SA = surface area

D = diameter

L = length

Example: (6,6) SWNT with the length of 7.44 nm

n, m = 6

L = 7.44

So, diameter of SWNT (D) = $\left(\frac{0.246}{\pi}\right)\left(6^2 + 6^2 + (6 \times 6)\right)^{1/2} = 0.8138$ nm.

So, surface area of SWNT (SA) = $\pi(0.8138)(7.44) = 19.0204$ nm^2.

Table A1 The diameters and surface areas of SWNTs

SWNT	Diameter (nm)	Surface area (nm^2)
(6,6)	0.8138	19.0204
(12,12)	1.6275	38.0408
(20,20)	2.7125	63.4014

Appendix B Calculation of the Number of SDBS Molecules in the Simulation System

Example: (6,6) SWNT with the length of 7.44 nm at the surface coverage of 2.8 molecules/nm^2 (0.357 nm^2/surfactant headgroup)

From

Surface coverage of SDBS on SWNT = 2.8 molecules/nm^2

Surface area of (6,6) SWNT = 19.0204 nm^2

So, the number of SDBS molecules on (6,6) SWNT

$$= \left(\frac{2.8 \quad \text{SDBS molecules}}{1 \quad nm^2 \quad \text{SWNT}} \right) \left(\frac{19.0204 \quad nm^2 \quad \text{SWNT}}{} \right)$$

= 53.26 SDBS molecules.

Table B1 The number of SDBS molecules on SWNTs at the surface coverages of 1.0 and 2.8 molecules/nm^2

SWNT	The number of SDBS molecules	
	Surface coverage of 1.0 molecules/nm^2	Surface coverage of 2.8 molecules/nm^2
(6,6)	19	53
(12,12)	38	106
(20,20)	63	178

Appendix C Calculation of the Effective SDBS Surface Coverage

The effective surface coverage of linear SDBS on the three SWNTs was computed from the time-average number of linear SDBS adsorbed on the SWNT by integrating the number density profiles of the linear SDBS molecules around the SWNT up to a cutoff distance of 12 Å (see Figure C1). The linear SDBS molecules located within the cutoff distance from the SWNT surface are considered to be adsorbed on the nanotube, and the linear SDBS molecules that are beyond the cutoff distance are considered as dispersed in the aqueous media (these can be found as monomers, and, sometimes, as small aggregates). The average number of SDBS not adsorbed is calculated at the difference between the total number of SDBS molecules present in the simulation box and the average number of SDBS molecules adsorbed on the nanotube.

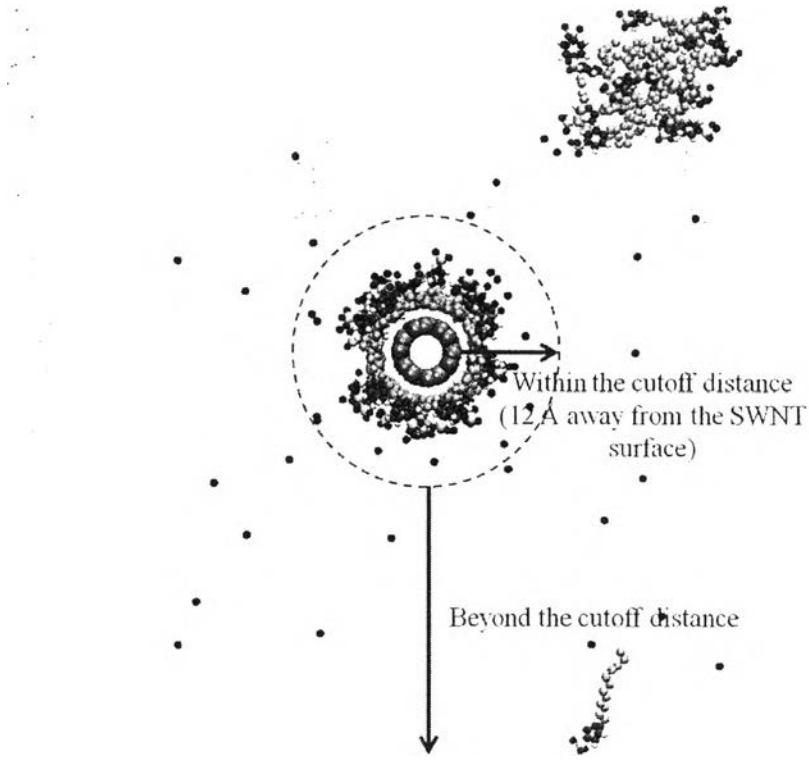

Figure C1 The SDBS adsorbed on the nanotube (within the cutoff distance) and the SDBS dispersed in aqueous media (beyond the cutoff distance).

Example: the average number of SDBS molecules adsorbed on the (6,6) SWNT with the length of 7.44 nm is 14 (the nominal surface coverage is 1.0 molecules/nm^2. 19 SDBS molecules).

From

Surface area of (6,6) SWNT = 19.0204 nm^2

Number of SDBS molecules (nominal surface coverage is 1.0 molecules/nm^2)

= 19 molecules

Average number of SDBS molecules adsorbed on the nanotubes

= 14 molecules

So, average number of non adsorbed SDBS

= 19.00 – 14.00

= 5.00 molecules.

So, effective surface coverage

$$= \left(\frac{14 \quad \text{SDBS molecules}}{19.0204 \quad nm^2 \quad \text{SWNT}} \right)$$

= 0.7361 molecules/nm^2

= 1.3585 nm^2/surfactant headgroup.

CURRICULUM VITAE

Name: Ms. Manaswee Suttipong

Date of Birth: January 3, 1987

Nationality: Thai

University Education:

2005–2009 Bachelor Degree of Engineering in Petrochemicals and Polymeric Materials, Faculty of Engineering and Industrial Technology, Silpakorn University, Thailand

Publication:

1. Suttipong, M.; Tummala, N.R.; Kitiyanan, B.; and Striolo, A. (2011) Role of surfactant molecular structure on self-assembly: Aqueous SDBS on carbon nanotubes. The Journal of Physical Chemistry C, submitted.

Presentations:

1. Suttipong, M.; Kitiyanan, B.; and Striolo, A. (2011, April 26) Molecular dynamics study of sodium dodecylbenzene sulfonate adsorption on single-walled carbon nanotubes. The 2st National Research Symposium on Petroleum, Petrochemicals, and Advanced Materials and The 17th PPC Symposium on Petroleum, Petrochemicals, and Polymers, Bangkok, Thailand.

2. Suttipong, M.; Thompson, J.R.; Tummala, N.R.; Kitiyanan, B.; and Striolo, A. (2011, March 21-25) Role of surfactant molecular structure on self-assembly: Aqueous SDBS on carbon nanotubes. The 2011 march Meeting of the American Physical Society, Dallas, Texas, USA.

Certificates:

1. Won "*First Prize Award of Poster Presentation*" at the 2011 march Meeting of the American Physical Society, Dallas, Texas, USA, 2011.

2. Won *"Grand Prize Award of Energy Efficiency Project"*, ESSO (Thailand) public company limited and ministry of energy, 2008.