Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information

Effects of Multivalent Counterions on the Morphology and Interactions of Carbon Nanotubes Grafted with Polyelectrolyte Chains

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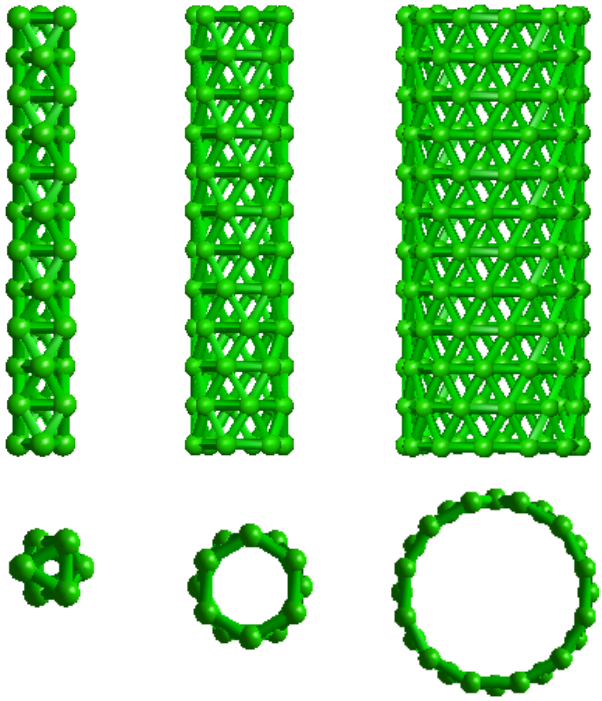

Figure S1. Side (top) and top (bottom) views of coarse-grained structures of SWNTs used in the simulations.

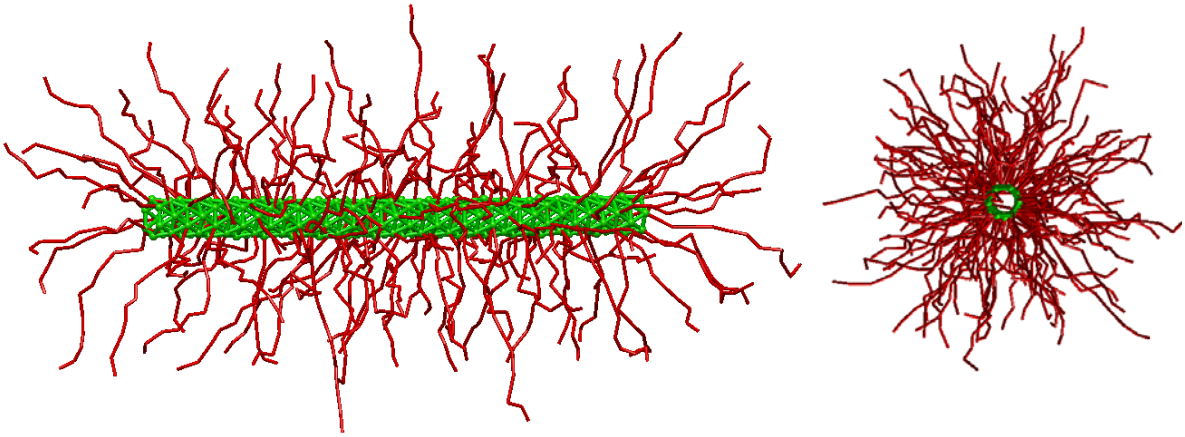

Figure S2. Side (left panel) and front views (right panel) of representative simulation snapshots for the grafted (12, 12) SWNT without added salt. The graft density of PE chains is α =0.025.Color scheme: (green) bonds and beads of CNT, (red) PE chains. Water and other ions are not shown for clarity.

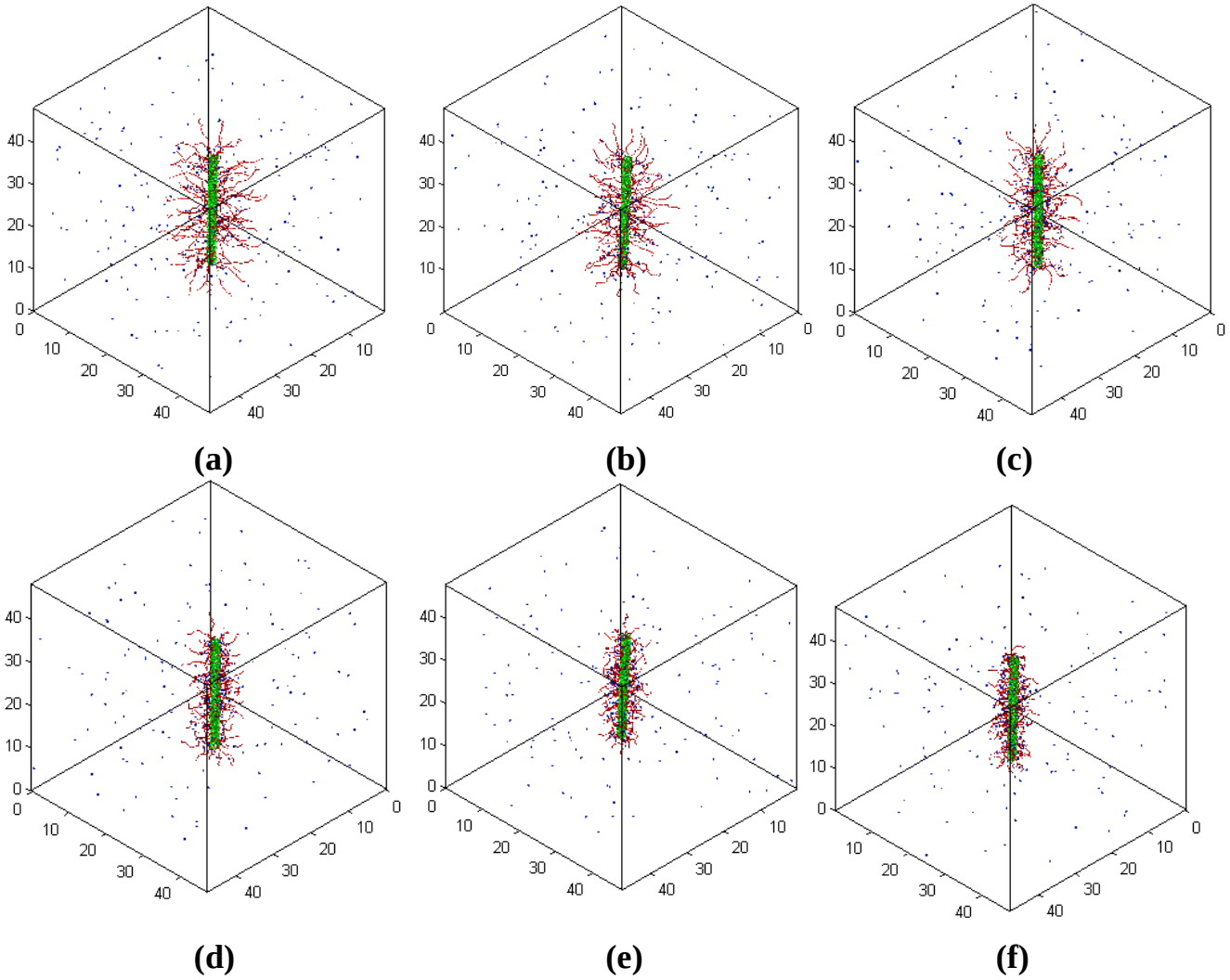

Figure S3. Conformational transition of PE chains grafted on a (12, 12) SWNT. The time at each snapshot is: t=0 μs (a), 0.004 μs (b), 0.039 μs (c), 0.117 μs (d), 0.176 μs (e) and 0.234 μs (f). The graft density of PE chains is α =0.025. Color scheme: (green) bonds and beads of CNT, (red) PE chains. The multivalent counterions are shown with small blue points. Water beads and other ions are not shown for clarity.

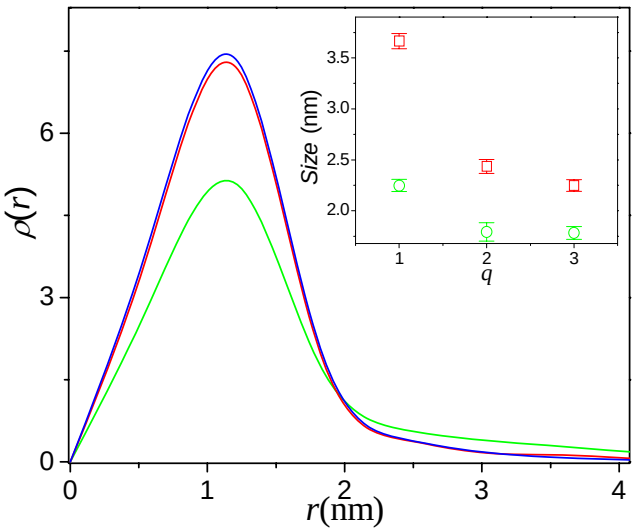

Figure S4. The radial density profiles for the PE chains grafting on the (12, 12) SWNT with various valencies of the counterions from added salt: (gree) q=1, (red) q=2 and (blue) q=3. The inset shows the thickness, L_c, (red) and the radius of gyration, R, (green) of the PE chains as a function of the counterion valency. The graft density of PE chains is α =0.008.

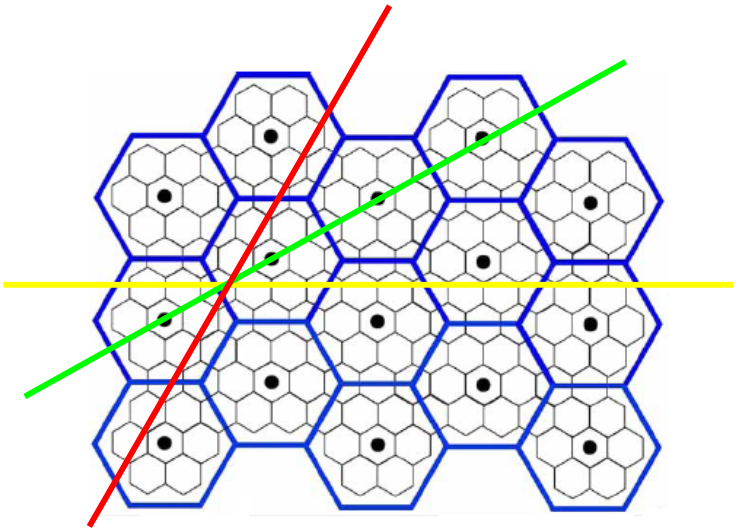

Figure S5. Schematic representation of the pitch angle threadlins of an armchair SWNT by grouping 24 carbon atoms. Solid dots represent the lumped beads while the thin black lines indicate the carbon-carbon bonds in the SWNT. The red and green lines denote the pitch angle threadlines of the atomistic and the coarse-grained models, respectively. The yellow line is the axis of the SWNT.

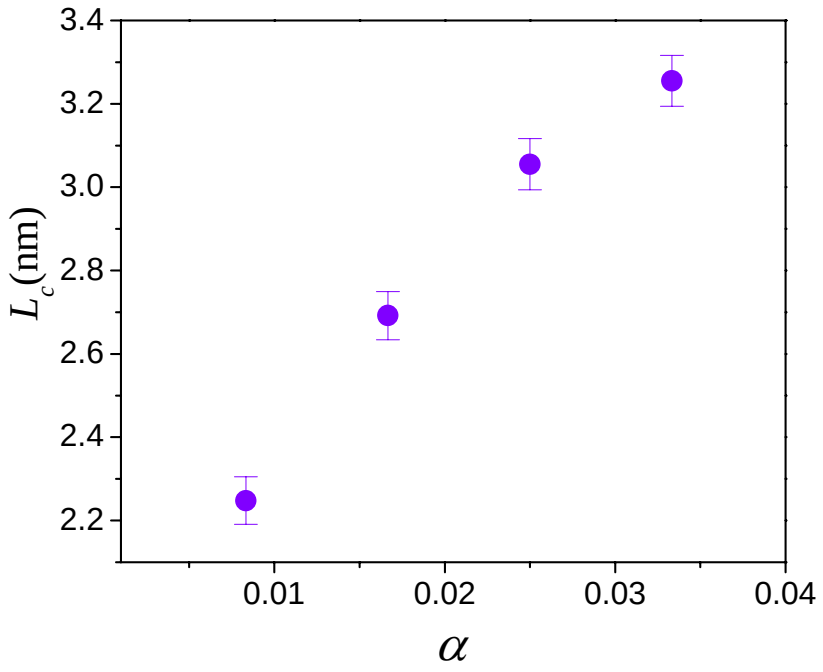

Figure S6. The thickness, L_c, of the PE chains as a function of the graft density α. The valency of the counterions from added salts is q=3.

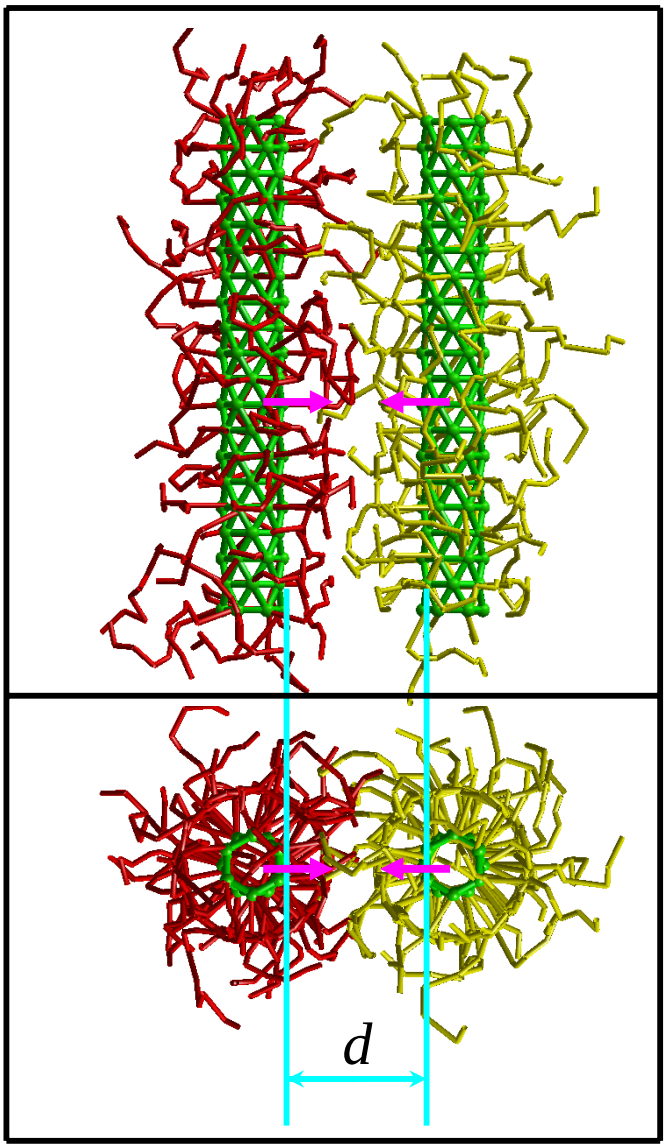

Figure S7. The side (top) and top (bottom) views of the configuration for two grafted SWNTs in the calculation of PMF. Color scheme: (green) bonds and beads of SWNT, (red) PE chains on the left SWNT and (yellow) PE chains on the right SWNT. Water and other ions are not shown for clarity. The pink arrows represent the moving direction of the SWNTs.

Table S1. The interaction parameter α_{ij} between different types of beads.

	Carbon atom in SWNT	PE chain	Monovalent ion from PE chain	Counterion from added salt	Monovalent ion from added salt	Solvent bead
Carbon atom in SWNT	25	15	80	80	80	80
PE chain	15	25	24	24	24	24
Monovalent ion from PE chain	80	24	25	25	25	25
Counterion from added salt	80	24	25	25	25	25
Monovalent ion from added salt	80	24	25	25	25	25
Solvent bead	80	24	25	25	25	25