Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

HRMAS-NMR and simulation study of self-assembly of surfactants on carbon nanotubes

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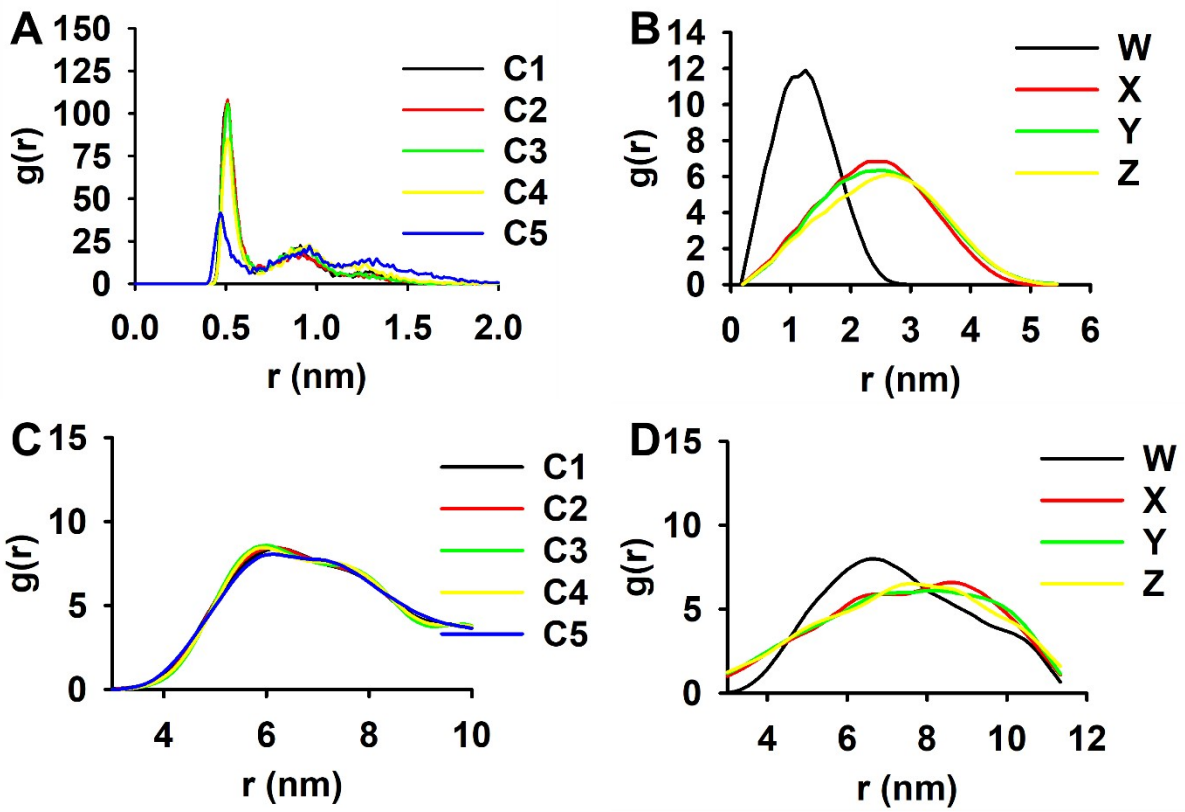
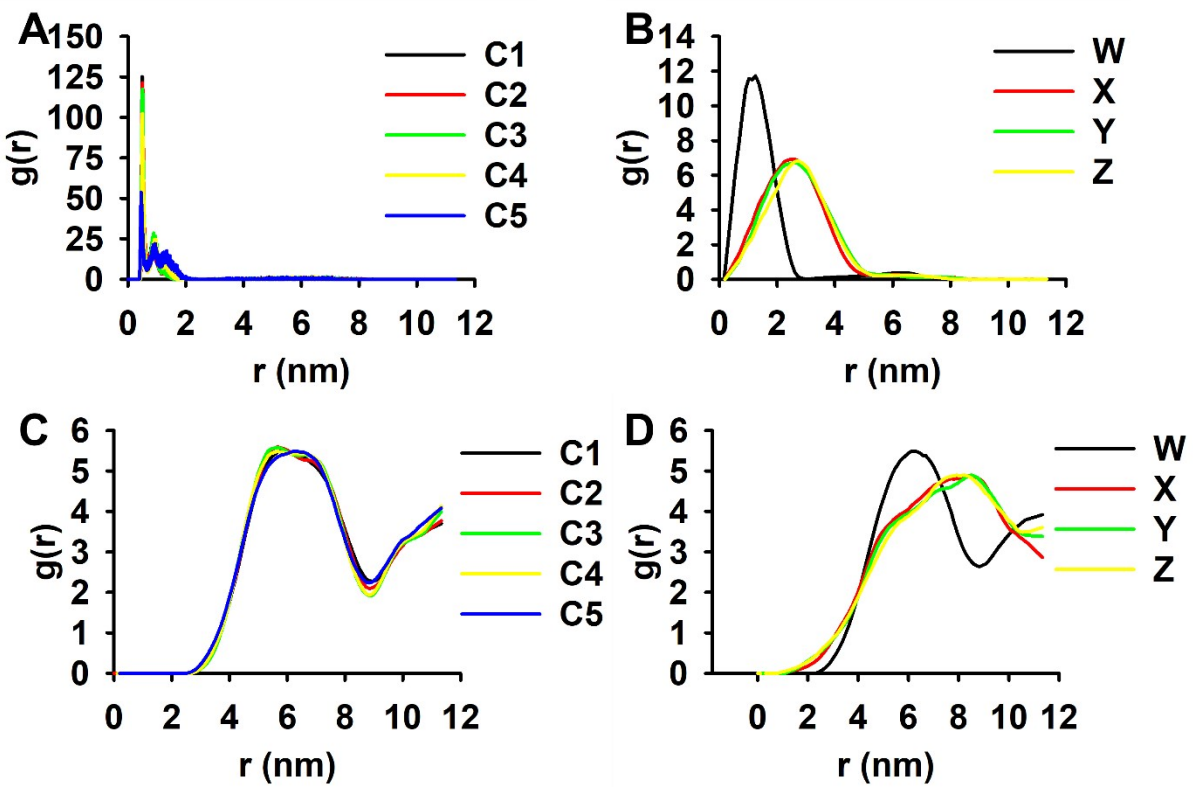
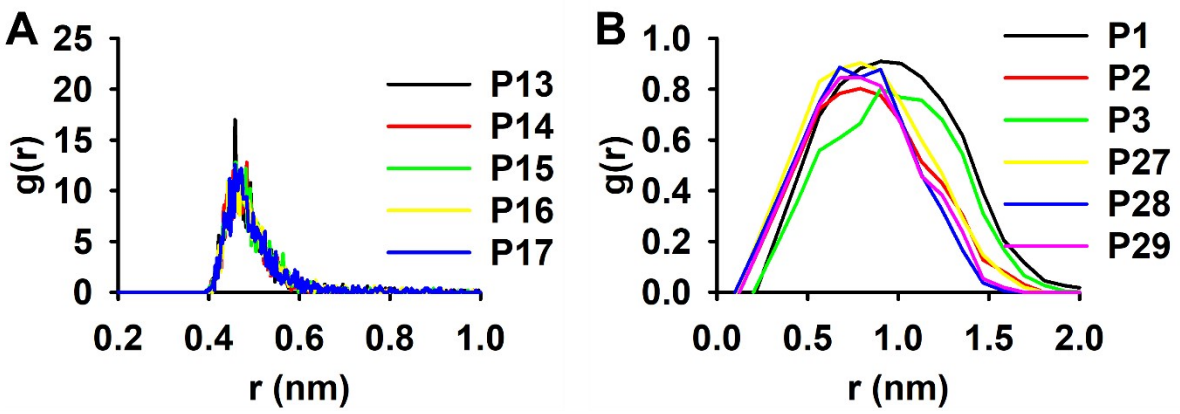


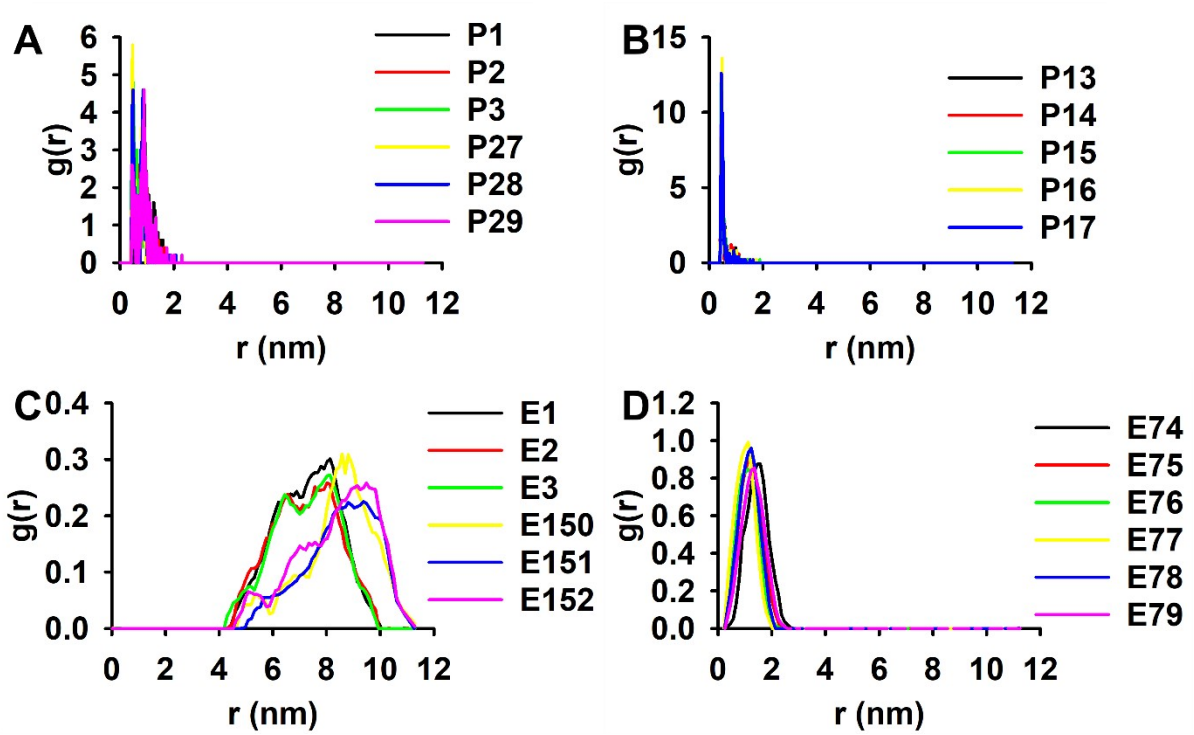
Supporting Figure S1. RDF between different beads in T80 molecules and SWCNT surface. (A, B) show RDF plots of different beads of SWCNT-bound micelle with SWCNT surface, (C, D) show RDF plots of different beads in unbound T80 molecules (micelles + unimers) with SWCNT surface. The RDF values in A-D were calculated for the last 50 ns of simulation from a total simulation time of 100 ns.



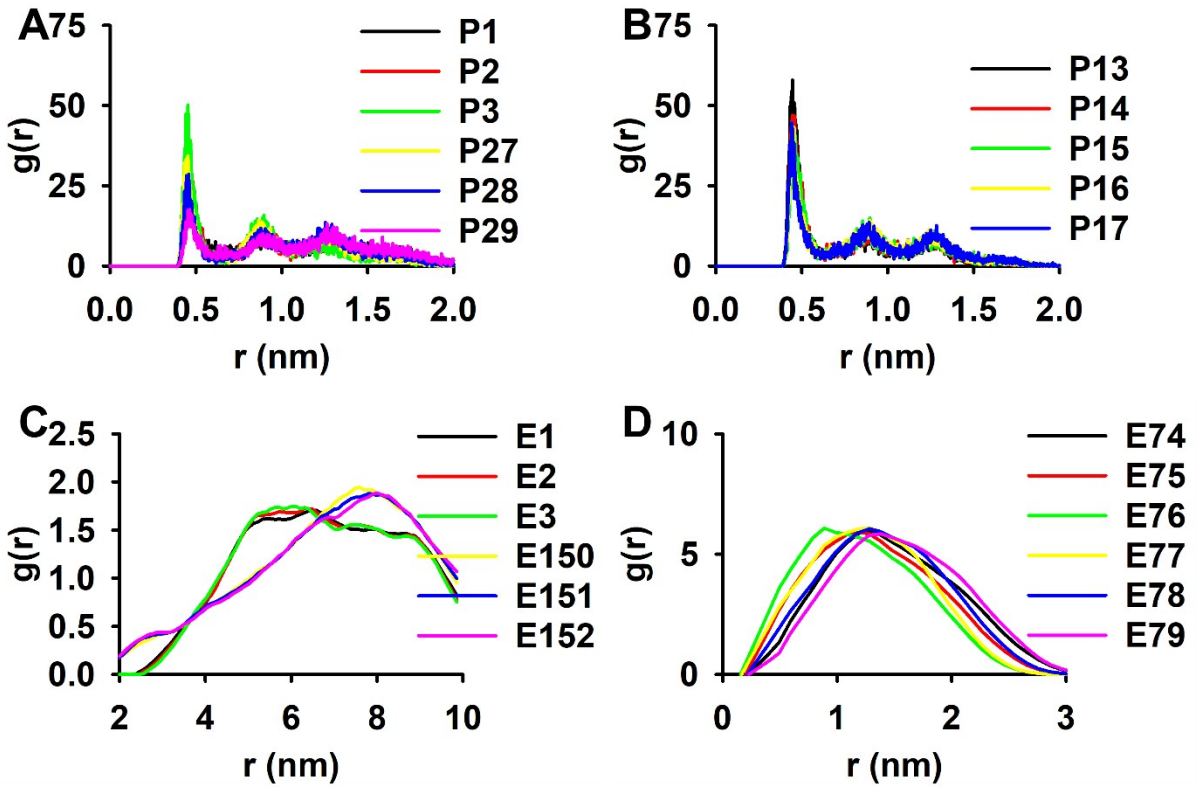
Supporting Figure S2. RDF between different beads in T80 molecules and SWCNT surface. (A, B) show RDF plots of different beads of SWCNT-bound micelle with SWCNT surface, (C, D) show RDF plots of different beads in unbound T80 molecules (micelles + unimers) with SWCNT surface. The RDF values in A-D were calculated for the last 50 ns of simulation from a total simulation time of 500 ns.



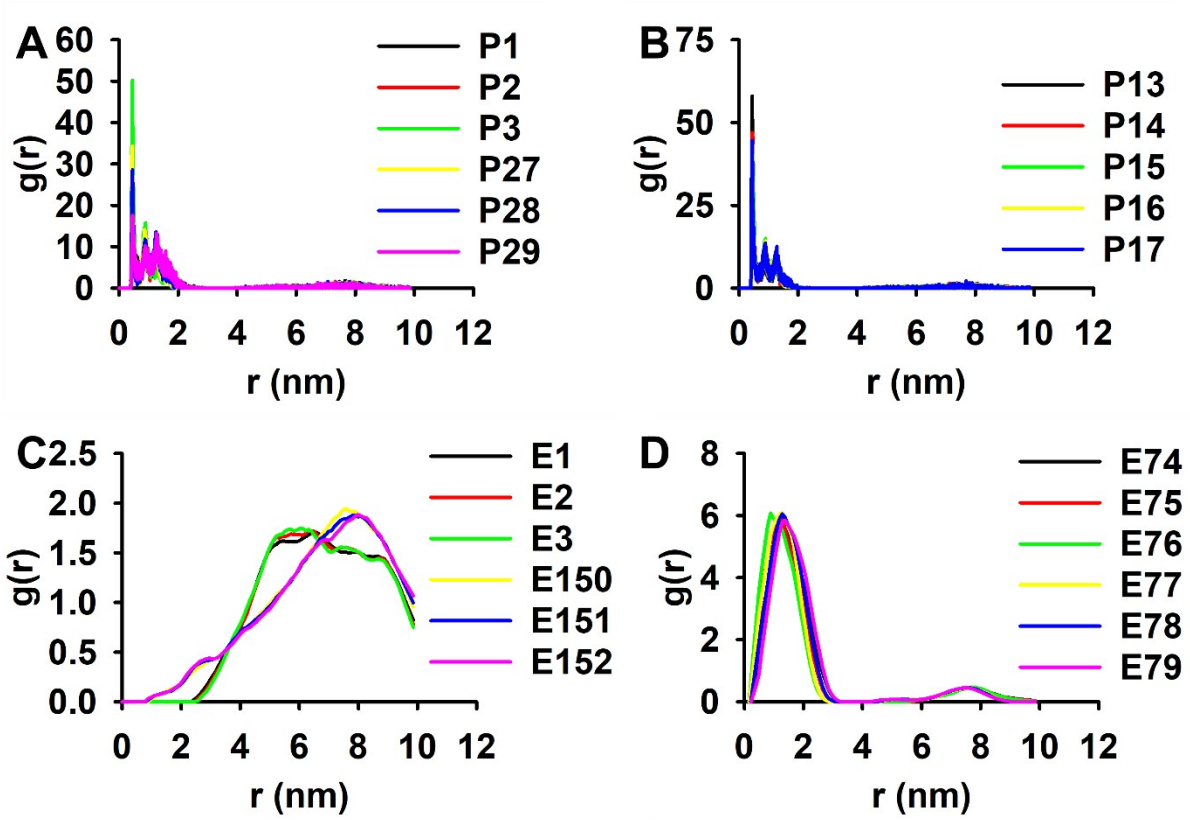
Supporting Figure S3. RDF between different beads in a PF68 molecule and SWCNT surface. (A, B) show RDF plots of PO beads with SWCNT surface. The interaction of a single PF68 molecule with SWCNT was studied. The RDF values in A and B were calculated for the last 50 ns of simulation from a total simulation time of 100 ns.



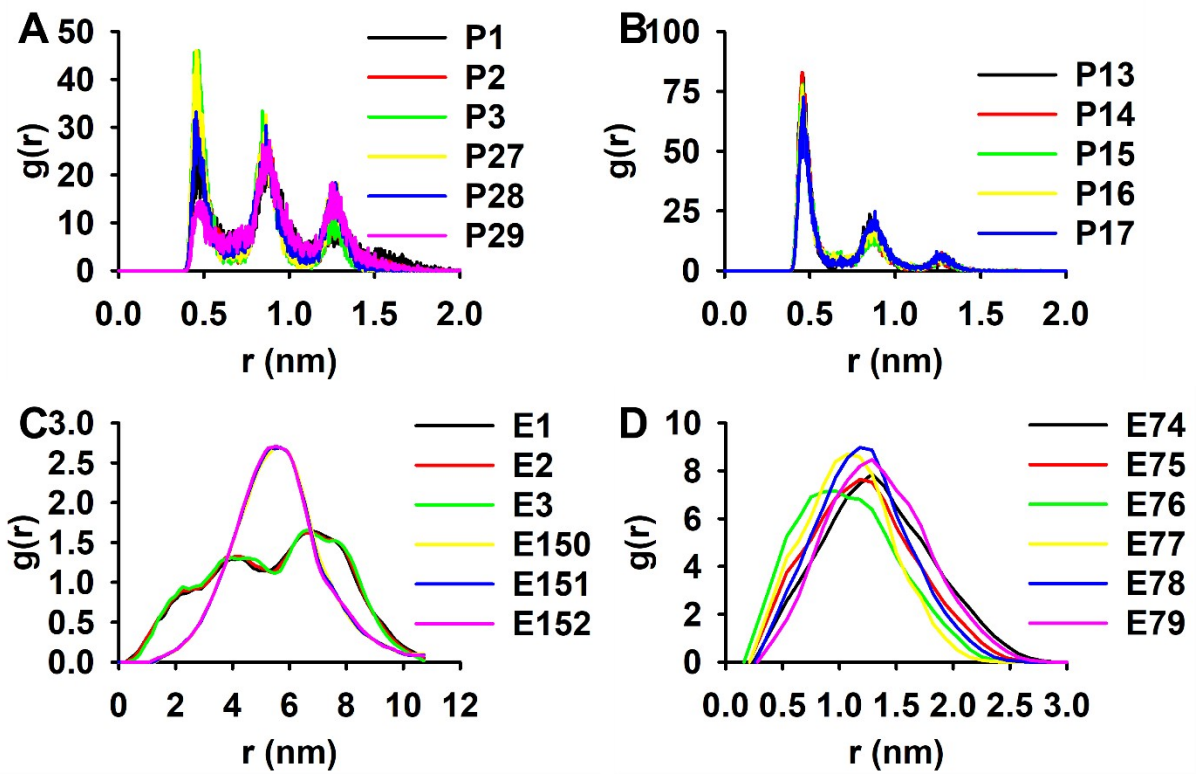
Supporting Figure S4. RDF between different beads in a PF68 molecule and SWCNT surface. (A, B) show RDF plots of PO beads with SWCNT surface while (C, D) show RDF plots of EO beads with SWCNT surface. The interaction of a single PF68 molecule with SWCNT was studied. The RDF values in A-D were calculated for the last 50 ns of simulation from a total simulation time of 500 ns.



Supporting Figure S5. RDF between different beads in 10 PF68 molecule and SWCNT surface. (A, B) show RDF plots of PO beads with SWCNT surface and (C, D) show RDF plots of EO beads with SWCNT surface. The interaction of 10 PF68 molecules with SWCNT was studied. The RDF values in A-D were calculated for the last 50 ns of simulation from a total simulation time of 100 ns.



Supporting Figure S6. RDF between different beads in 10 PF68 molecule and SWCNT surface. (A, B) show RDF plots of PO beads with SWCNT surface and (C, D) show RDF plots of EO beads with SWCNT surface. The interaction of 10 PF68 molecules with SWCNT was studied. The RDF values in A-D were calculated for the last 50 ns of simulation from a total simulation time of 500 ns.



Supporting Figure S7. RDF between different beads in 10 PF68 molecule and MWCNT surface. (A, B) show RDF plots of PO beads with MWCNT surface and (C, D) show RDF plots of EO beads with MWCNT surface. The interaction of 10 PF68 molecules with MWCNT was studied. The RDF values in A-D were calculated for the last 50 ns of simulation from a total simulation time of 100 ns.