Supporting Information for

Molecular dynamics simulations on fullerene surfactants with different charges at the air-water interface

Yunzhi Li[a,1], Yaoyao Wei[a,1], Xia Leng[a], Guokui Liu[a,*], Qiying Xia[a,*], Honglei Wang[b,*]

[a] School of Chemistry and Chemical Engineering, Linyi University, Linyi 276000, China

[b] Beijing Kein Research Center for Natural Sciences, Beijing 100022, China

* Corresponding authors.
E-mail addresses: liuguokui@lyu.edu.cn (G. Liu), xiaqiying@lyu.edu.cn (Q. Xia), wanghl@qibebt.ac.cn (H. Wang)
[1] Both authors contribute equally to this work.

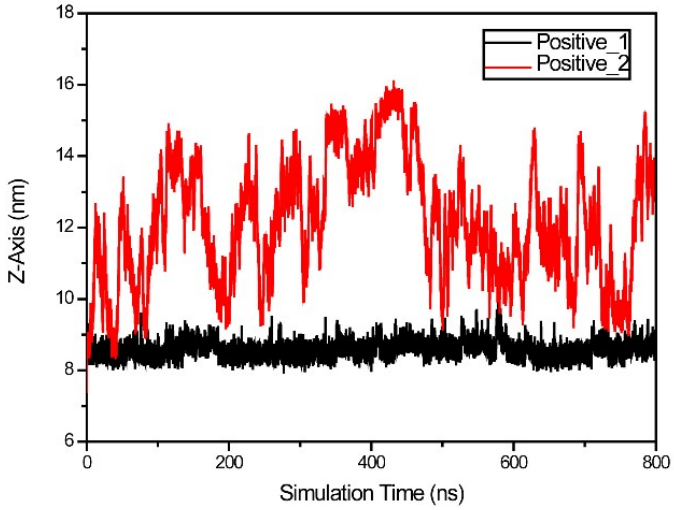

Fig. S1 The Z-direction location of fullerene surfactants COM with the time evolution of 800 ns.

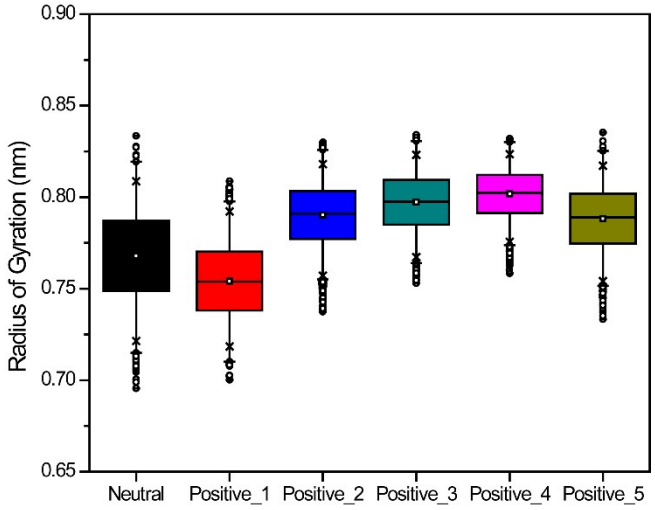

Fig. S2 The radius of gyration for different surfactants.

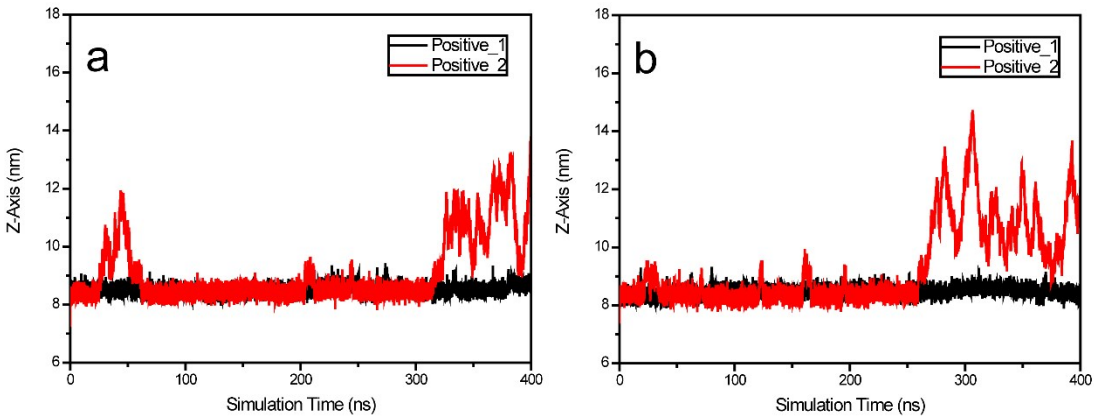

Fig. S3 The z-location of Positive_1 and Positive_2 surfactants COM with the time evolution using different water models (a: TIP4P; b: TIP5P).

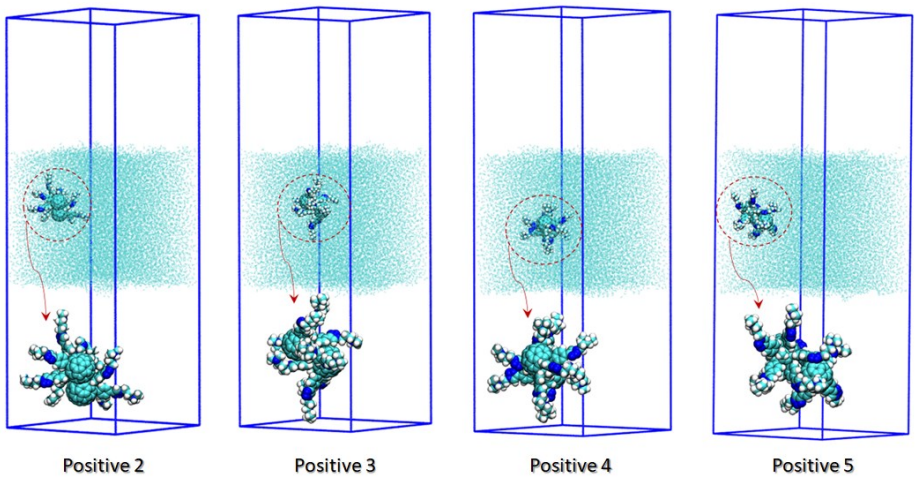

Fig. S4 Snapshots of aggregation structures for Positive_2, Positive_3, Positive_4 and Positive_5.

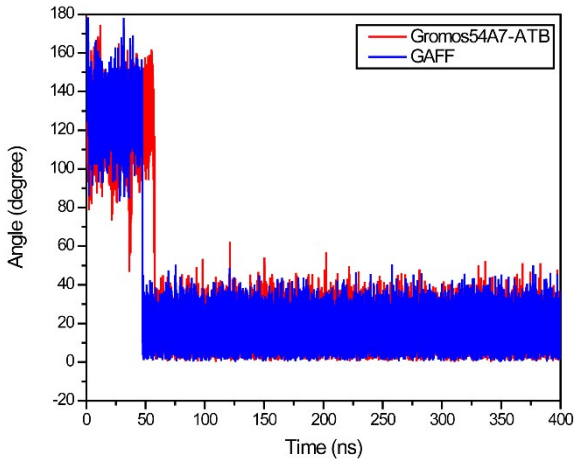

Fig. S5 The angle distribution of Neutral with different force fields (GAFF stands for the generalized Amber force field, and Gromos54A7-ATB stands for the force field generated with the Automated Topology Builder).