Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2018

Dual Hydrophobic Grafted Chains Facilitating Quaternary Ammonium Aggregations of Hydroxide Conducting Polymers: A Theoretical and Experimental Investigation

Jin Ran[*1,2], Cenfeng Fu[3], Liang Ding[2], Pengrui Cao[1] and Tongwen Xu[*2]

1. School of Chemistry and Chemical Engineering, Hefei University of Technology Hefei, Anhui 230009, People's Republic of China

2. CAS Key Laboratory of Soft Matter Chemistry, Lab of Functional Membranes, School of Chemistry and Material Science, University of Science and Technology of China, Hefei 230026, P.R. China;

3. Department of Chemical Physics, School of Chemistry and Material Science, University of Science and Technology of China, Hefei 230026, P.R. China

***Corresponding author. Tel: +86(551)-63601587; E-mail:** twxu@ustc.edu.cn, ranjin@mail.ustc.edu.cn**.**

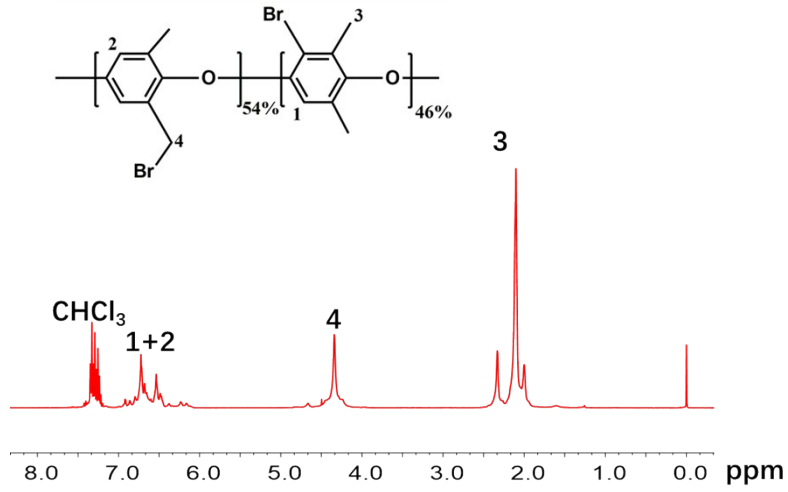

Figure S1. ^{1}H NMR of BPPO in $CDCl_3$.

Table S1. The added amine amounts for targeted products.

Sample	C6C6-X20Y30	C6C6-X30Y20	C6C6-X40Y10	C10C6-X20Y30	C10C6-X30Y20	C10C6-X40Y10	C16C6-X20Y30	C16C6-X30Y20	C16C6-X40Y10
Amine (g)	0.143	0.214	0.285	0.205	0.307	0.409	0.297	0.446	0.595

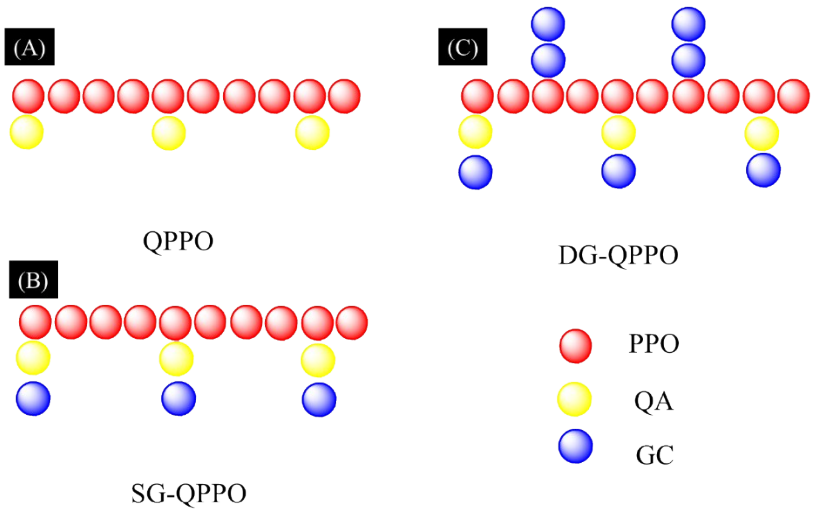

Figure S2. The models used for the calculated system (A) QPPO; (B) SG-QPPO; (C) DG-QPPO. Note that one PPO bead corresponds to one PPO monomer unit

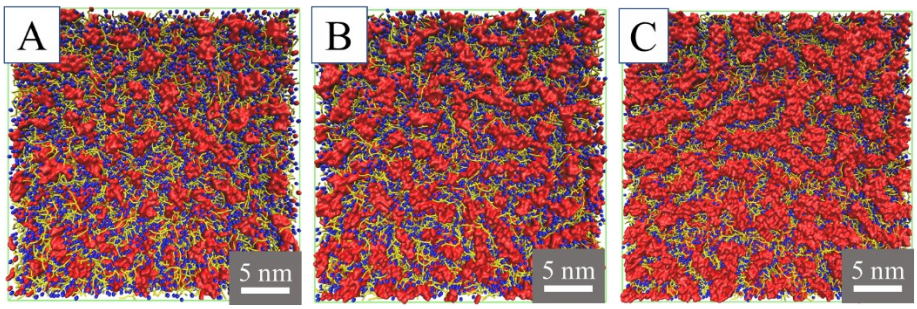

Figure S3. The collected snapshots of the computed results of (A) C6C6; (B) C10C6; (C) C16C6. Yellow represents PPO domains; Blue represents QA and OH domains; Red represents GC domains.

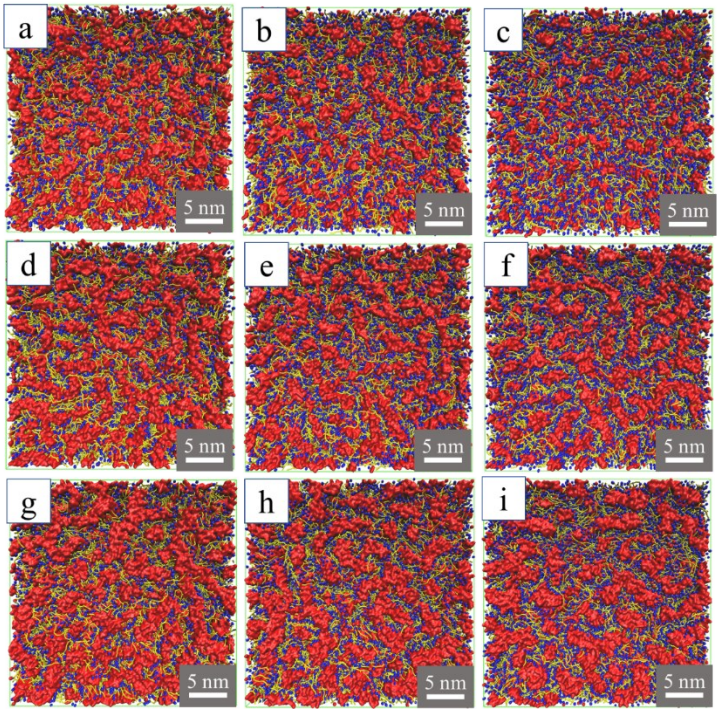

Figure S4. The collected snapshots of the computed results of (a) C6C6-X20Y30; (b) C6C6-X30Y20; (c) C6C6-X40Y10; (d) C10C6-X20Y30; (e) C10C6-X30Y20; (f) C10C6-X40Y10; (g) C16C6-X20Y30; (h) C16C6-X30Y20; (i) C16C6-X40Y10. Yellow represents PPO domains; Blue represents QA and OH domains; Red represents GC domains.

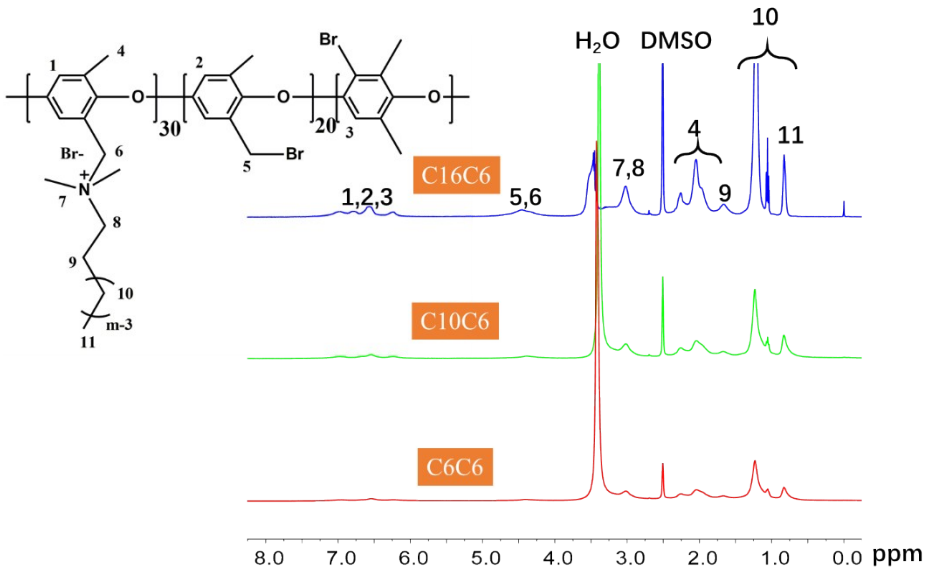

Figure S5. ^{1}H NMR spectra of SG-QPPO polymers in d-DMSO.