Supplementary Material

Water Structure Change-Induced Expansion and Collapse of Zwitterionic Polymers Surface-Grafted onto Carbon Black

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contents:

calculation of surface grafting density using the results of the chemical analysis

Data

Sample	C [w/w%]	N [w/w%]	S [w/w%]	Br [w/w%]
Bare CB	45.14	0.44	—	—
CB-Br	48.46	9.24	—	20.8
CB-PMPDSAH	40.29	5.18	0.97	3.32

compositions

	MW	C	N	S	Br
initiator	236.9	7	1	0	1
initiator -Br	157	7	1	0	0
monomer	292	12	2	1	0

deduced mole ratios and masses (100g of sample)

	mol initiator from Br	mol initiator from N	mass initiator from Br	mole initiator - Br	mass initiator-Br	total initiator mass	mol C in initiator from N	mass C in initiator from N
CB-Br	0.260325	0.66	61.67109	0.399675	62.74891	124.42 should be <100	4.62	55.44

	mol monomer from S	mol N	mol polymer and unreacted initiator from Br	mol N in monomer from S	mol N as unreacted initiator	mol C as unreacted initiator	mol C in monomer from S	total mass C in polymer and initiator	mass of carbon as CB
CB-PMPDSAH	0.03	0.37	0.04	0.06	0.31	2.17	0.36	30.35	9.94

polymer yield

mass of initiator-loaded C	added mass	total mass if all reacted	%S if all reacted	yield of polymer (from S)
0.20	1.25	1.45	10.96	8.9%

Carbon nanopowder particle specification

assay	≥99% trace metals basis
form	nanopowder
particle size	<50 nm (TEM)
spec. surface area >100 m2/g (BET)	
amorphous carbon	

density of amorphous carbon
1.8-2.1g/cm^3

Deduced polymer coverage on carbon surface

assumed radius	assumed MW of polymer	mole particle/100g CB-PMPDSAH	monomer/particle from S	polymer / particle
20nm	10000 (34 units)	2.5E-07	1.2E+05	12.3
10nm	10000 (34 units)	2.0E-06	1.5E+04	1.5