

Supporting information

Morphology-controlled synthesis of porous polymer nanospheres for gas absorption and bioimaging applications

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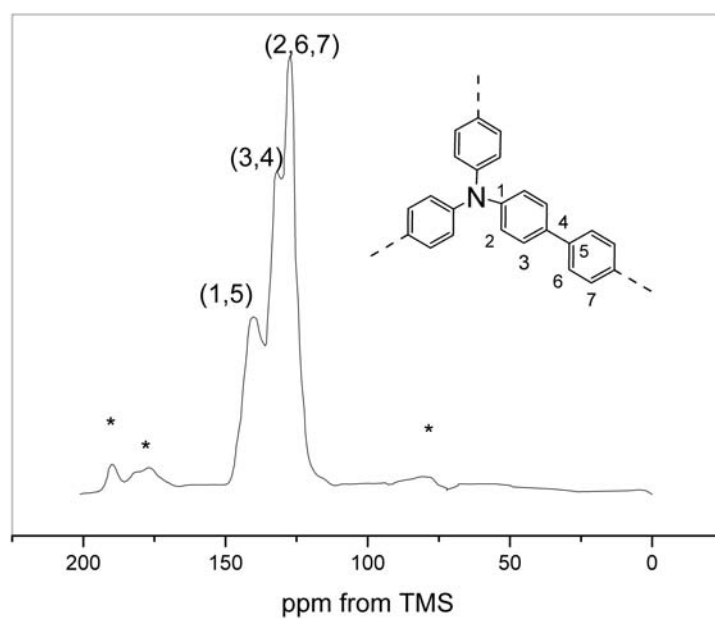
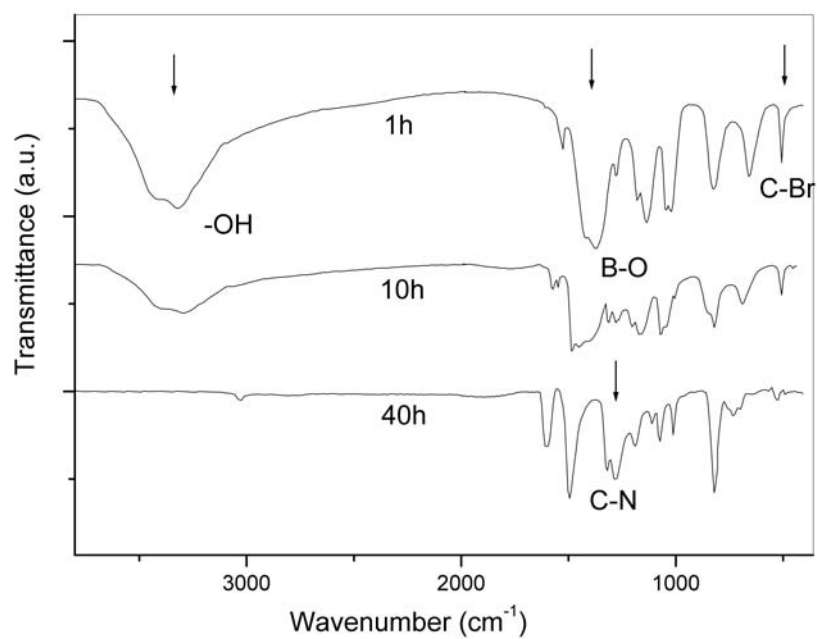


Figure S1. ^{13}C CP/MAS NMR spectrum of the PPS with a reaction time of 40 h. Asterisks denote spinning sidebands.



FigureS2 . FTIR spectra of PPSs with different reaction times.

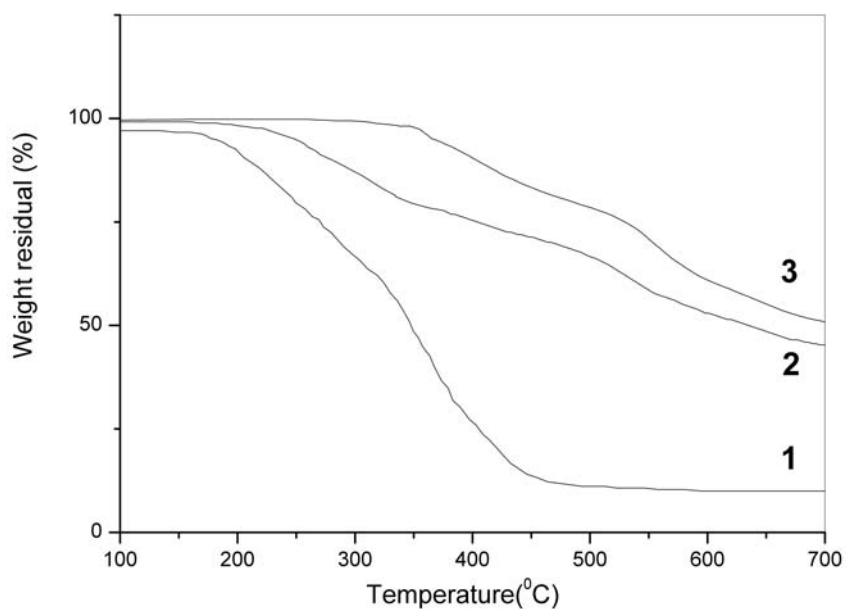


Figure S3 . TGA curves recorded under N₂ for PPSs with different reaction times: (1) 10 h, (2) 30 h and (3) 40 h.

Theoretical Calculations.

All periodic DFT calculations were performed using SIESTA code with numerical-orbital basis sets. The exchange-correlation functional used is the generalized gradient-approximation method, known as GGA-PBE. A double-plus polarization basis set was employed. The orbital confining cutoff radii were determined from an energy shift of 0.01 eV. The energy cutoff for the real space grid used to represent the density was set as 150 Ry. To further speed up calculations, Kohn-Sham equation was solved by an iterative parallel diagonalization method that utilizes the ScaLAPACK subroutine pdsygvx with two-dimensional block cyclicly distributed matrix. The accuracy of the SIESTA method was carefully benchmarked with the plane-wave code used previously.

	d _{N···N} (Å) nearest d	d _{N···N} (Å), diagonal d	
	14.327	28.930	
	14.099	25.777	
	14.353	28.823	
	14.291	30.300	
	14.285	25.829	
	14.267	28.510	
	14.312	29.146	
	14.376	27.467	
	14.360	28.405	
	14.308	27.155	
	14.134	28.916	
	14.348	29.049	
	14.306	28.374	
	14.304	29.054	
	14.175	27.951	
	14.239	28.779	
	14.231	28.202	
	14.262	28.288	
	14.304	28.896	
	14.282	28.059	
	14.250	27.560	
	14.282	28.260	mean
	14.207	0.7699	dev
	14.241	30.300	max
	14.306	25.777	min
7pore	14.224		
1056 atoms	14.076		
COMPASS (ultrafine)	14.363		

	14. 316		
	14. 246		
mean	14. 269		
dev	0. 0565		
max	14. 376		
min	14. 076		

