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

Electronic Supplementary Information for

Influence of Applied Silica Nanoparticles on Bio-renewable Castor Oil Based Polyurethane Nanocomposite and its Physicochemical Properties

Kamal Mohamed Seeni Meera,[a] Rajavelu Murali Sankar,[a] Jaya Paul,[a]
Sellamuthu N Jaisankar,[a] and Asit Baran Mandal*[,a,b]

[a]Polymer Division, Council of Scientific and Industrial Research (CSIR) –
Central Leather Research Institute (CLRI), Adyar, Chennai 600020, Tamil Nadu, India.
[b]Chemical Laboratory, Council of Scientific and Industrial Research (CSIR) –
Central Leather Research Institute (CLRI), Adyar, Chennai 600020, Tamil Nadu, India.

**Corresponding author: E-mail: abmandal@hotmail.com; abmandal@clri.res.in*
Tel.: +91-44-24910846/0897; Fax: +91-44-24912150.

FT-IR spectra of silica nanoparticles

The FT-IR spectra of unmodified (UMS) and amine modified (AMS) silica nanoparticles were given in Fig. S1. The spectrum of UMS gives a peak at 3347 cm^{-1} corresponds to -OH groups present in the surface of silica nanoparticles. Further, Si-O and O-Si-O stretching vibrations appear at 1060 and 790 cm^{-1}, respectively. In the case of AMS, some new peaks were appeared apart from characteristic UMS particles. The N-H vibration of APTMS appears at around 1655 cm^{-1} and the C-H vibration appears in the range of 2978-2748 cm^{-1} for the amine modified silica nanoparticles.[1] From the FT-IR results, it can be concluded that surface of silica nanoparticle successfully functionalized with amine groups.

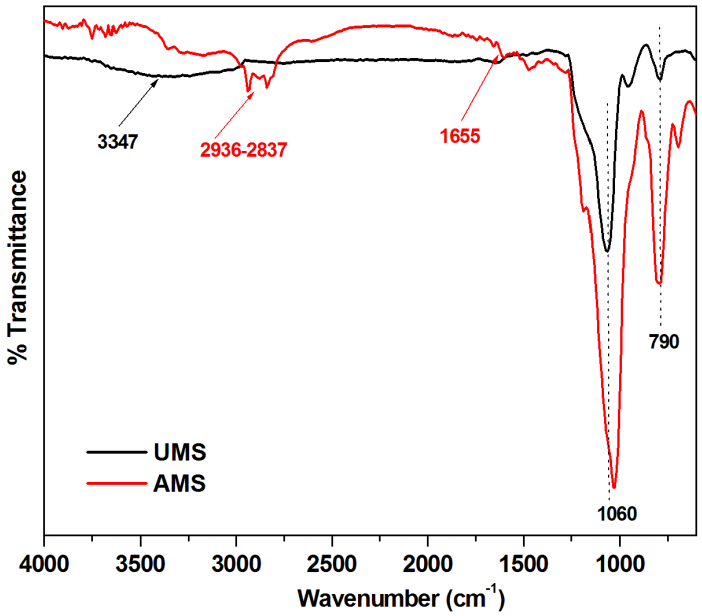

Fig. S1 FT-IR spectra for the prepared nanoparticles.

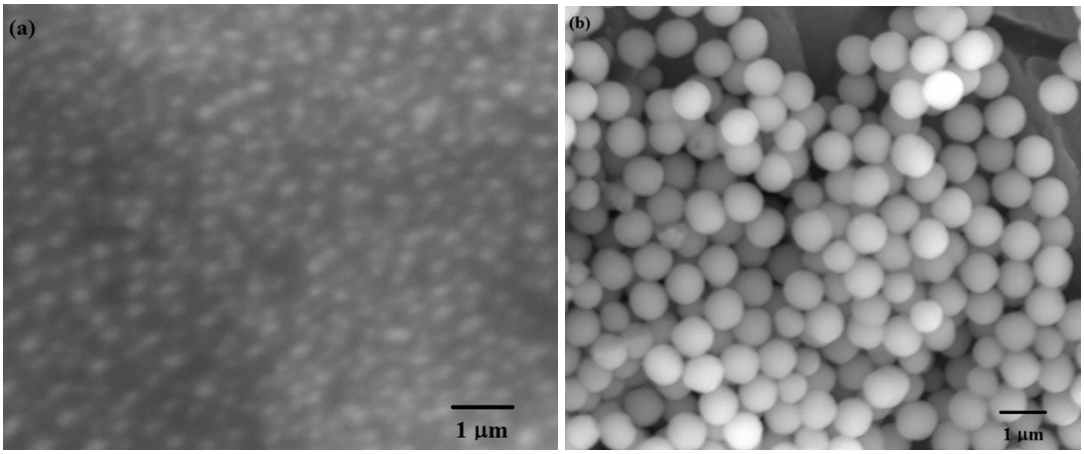

Fig. S2 SEM images of (a) UMS and (b) AMS.

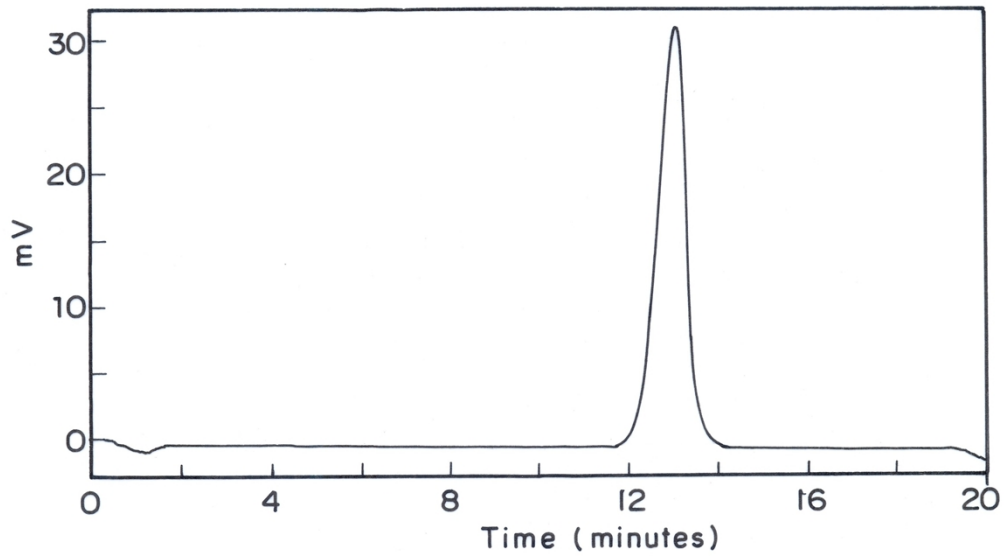

Fig. S3 GPC traces of prepared castor oil polyurethane.

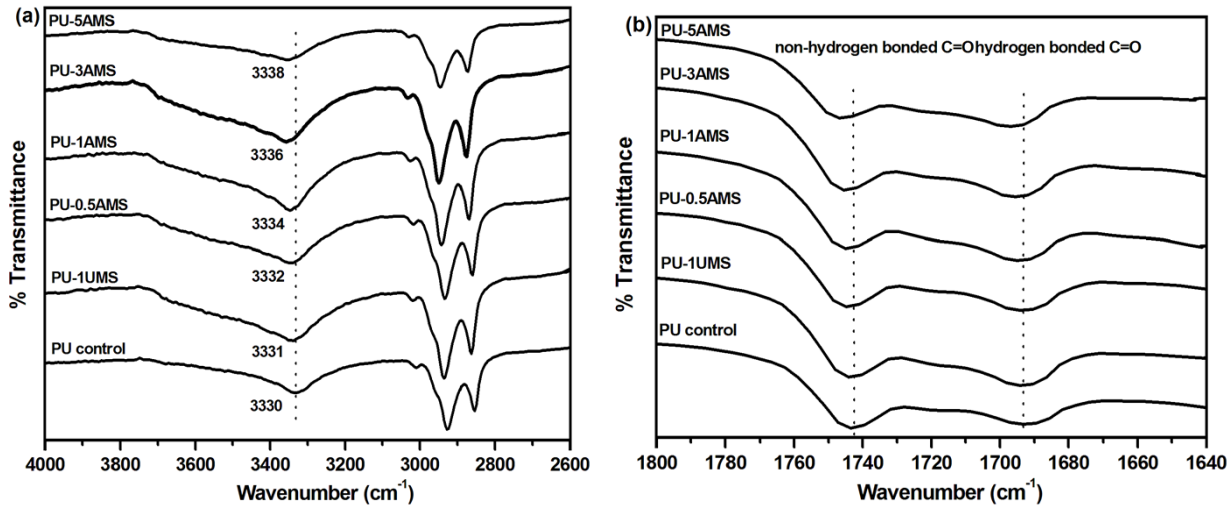

Fig. S4 ATR-FTIR spectra for the expanded regions of PU nanocomposite films: (a) N-H [4000-2600 cm^{-1}] and (b) C=O [1800-1640 cm^{-1}] regions.

Table S1 Characteristics of N-H and C=O regions in the IR spectra of nanocomposite sample at different concentration of nanoparticles.

Codes	N-H region (cm^{-1})	C=O region (cm^{-1})	
		hydrogen bonded	non-hydrogen bonded
PU control	3330.2	1692.4	1741.8
PU-1UMS	3331.4	1692.7	1742.4
PU-0.5AMS	3332.3	1693.4	1743.1
PU-1AMS	3333.6	1694.2	1744.6
PU-3AMS	3336.2	1696.1	1745.2
PU-5AMS	3338.1	1697.8	1746.2

Table S2 Thermogravimetric data for castor oil polyurethane/silica nanocomposite films.

Codes	1st stage degradation temperature T_{max1} (°C) at different heating rates (°C/min)				2nd stage degradation temperature T_{max2} (°C) at different heating rates (°C/min)			
	5	10	15	20	5	10	15	20
PU control	339	353	362	371	442	455	475	481
PU-1UMS	347	358	363	375	444	458	477	483
PU-0.5AMS	348	364	368	372	443	457	478	484
PU-1AMS	350	365	372	376	445	459	480	485
PU-3AMS	351	367	373	380	447	461	482	487
PU-5AMS	353	368	377	381	449	469	483	489

Table S3 Thermal properties of polyurethane/silica nanocomposite films at a heating rate of 5 °C/min.

Codes	Temperature at mass loss (°C)			Residue (%)
	5%	10%	50%	
PU control	271.1	292.6	354.4	0.003
PU-1UMS	287.8	302.6	355.3	0.006
PU-0.5AMS	291.5	303.7	355.8	0.009
PU-1AMS	292.5	305.4	362.1	2.934
PU-3AMS	294.8	307.7	364.2	5.511
PU-5AMS	295.9	308.4	366.1	8.228

Table S4 Weight loss behavior for the castor oil polyurethane/silica nanocomposite films.

Codes	% decomposition up to 350 °C at different heating rates (°C/min)				% of decomposition up to 450°C at different heating rates (°C/min)			
	5	10	15	20	5	10	15	20
PU control	46.9	31.9	23.6	18.2	91.1	81.3	72.6	72.1
PU-1UMS	44.4	31.7	22.9	16.1	92.5	80.6	73.8	71.2
PU-0.5AMS	46.7	30.4	21.7	14.8	94.2	83.8	74.7	68.2
PU-1AMS	40.4	27.6	20.3	16.9	87.7	78.6	71.3	62.4
PU-3AMS	38.3	29.9	22.4	16.4	86.6	85.9	70.8	63.9
PU-5AMS	39.9	28.3	22.3	16.1	83.7	68.3	72.6	61.8

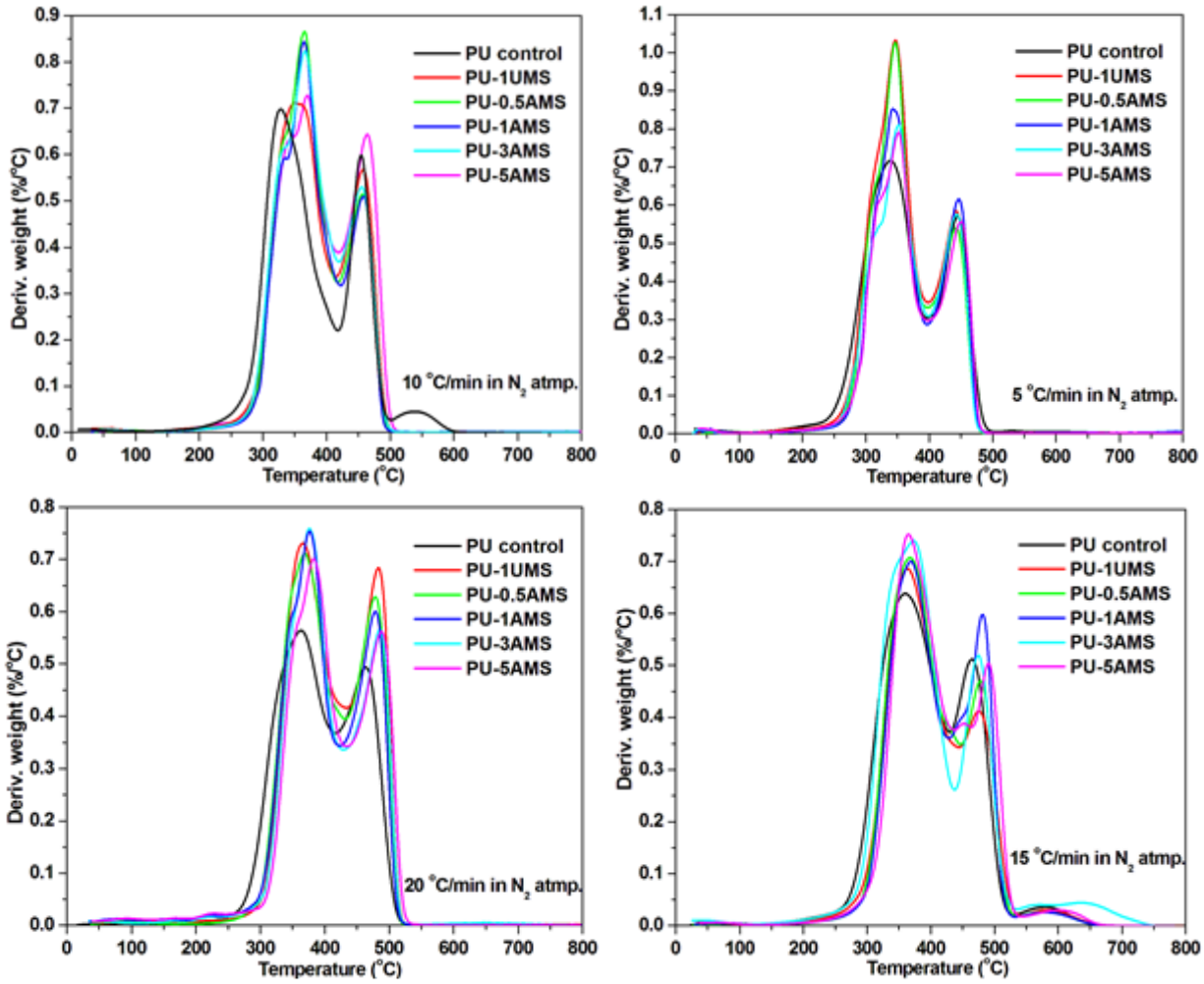

Fig. S5 Derivative thermograms for the polyurethane/silica nanocomposite films taken at different heating rates.

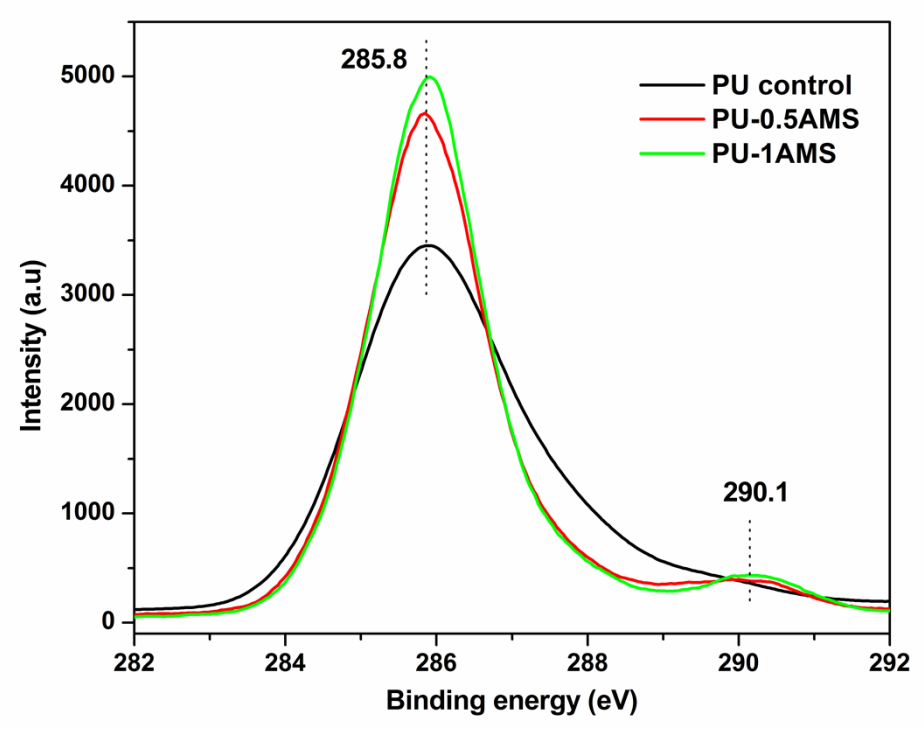

Fig. S6 XPS spectra of C_{1s} of PU and Nanocomposites.

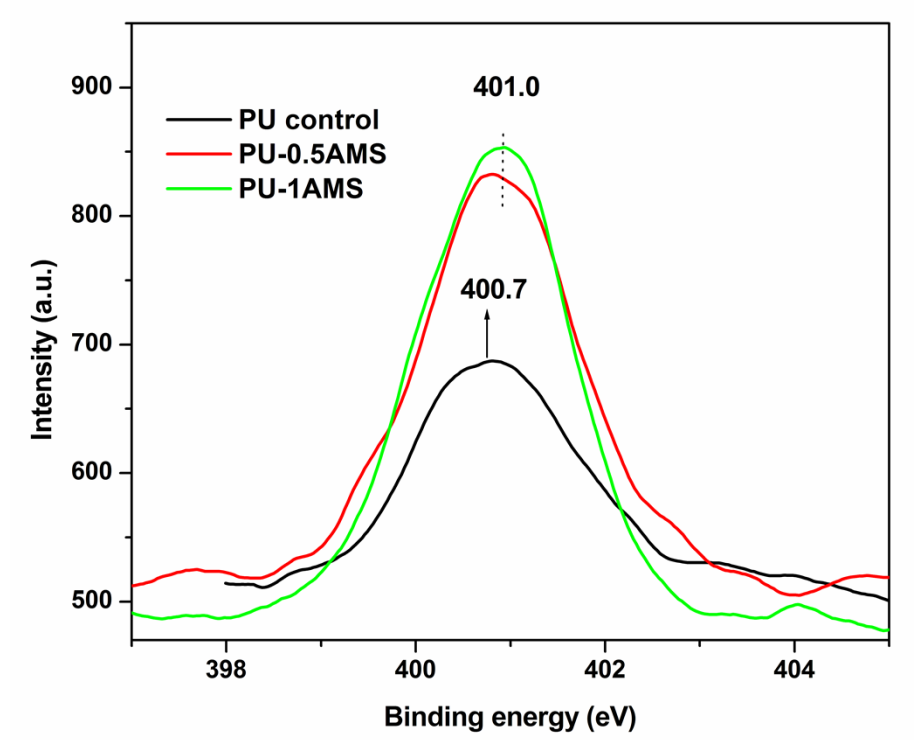

Fig. S7 XPS spectra of N_{1s} of PU and Nanocomposites.

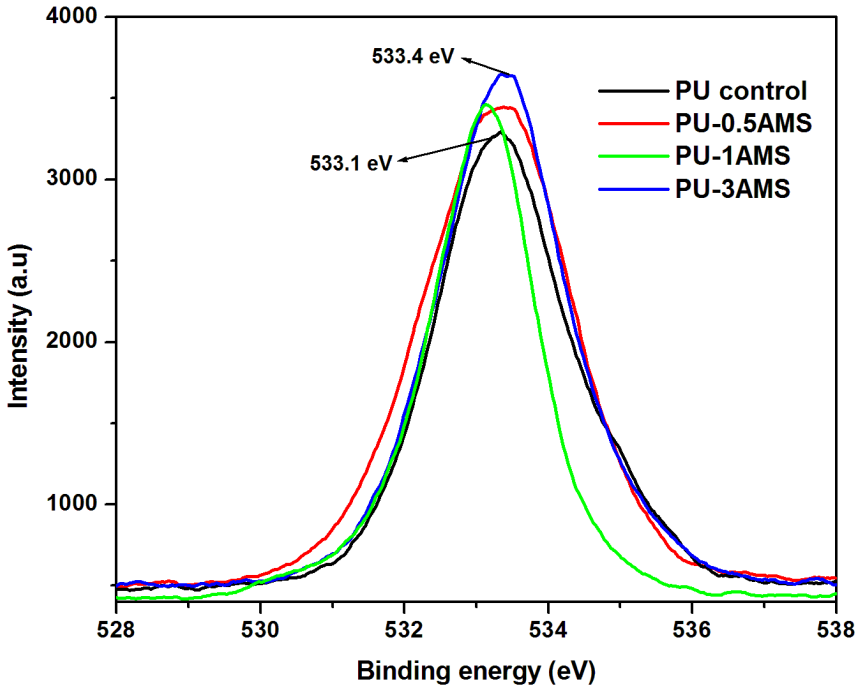

Fig. S8 XPS spectra of O_{1s} of PU and Nanocomposites

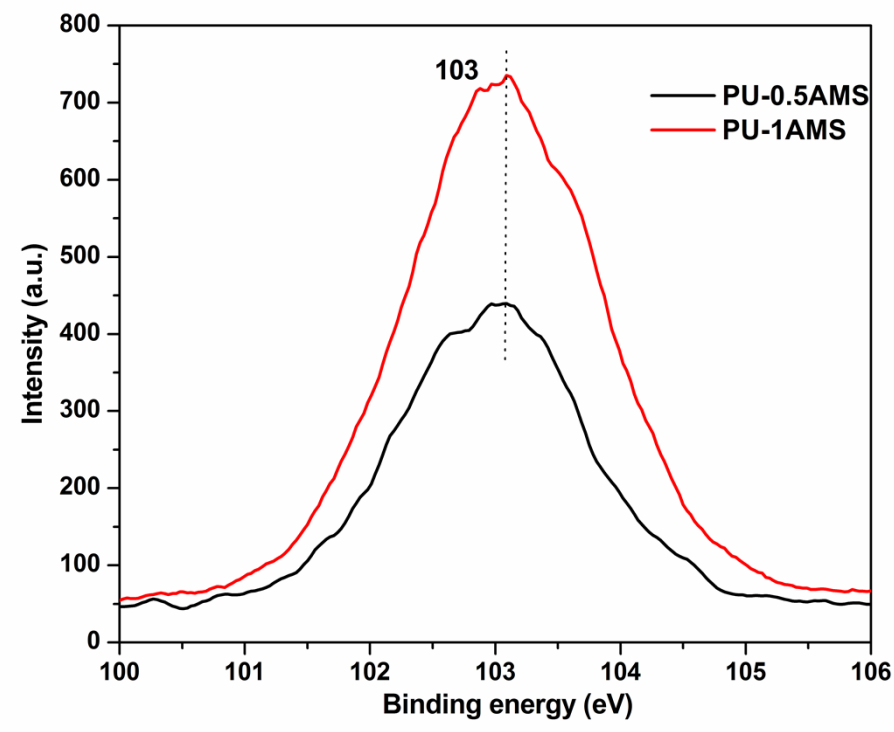

Fig. S9 XPS spectra of Si_{1s} of Nanocomposites.

Table S5 Mechanical properties for the prepared polyurethane/silica nanocomposites.

Codes	Tensile Strength (MPa)	Young's Modulus (MPa)	Elongation at break (%)
PU control	3.7 ± 0.8	1.6±0.1	67.0 ± 10.2
PU-1UMS	4.5 ± 1.0	1.7±0.1	68.1 ± 15.8
PU-0.5AMS	3.9 ± 1.0	1.8±0.1	67.2 ± 11.5
PU-1AMS	6.3 ± 0.7	2.2±0.1	83.5 ± 15.1
PU-3AMS	3.2 ± 0.6	2.3±0.1	40.9 ± 13.8
PU-5AMS	4.4 ± 0.7	2.4±0.1	64.3 ± 13.4

References

1 Y. Sun, Z. Zhang and C. P. Wong, *J. Colloid Interface Sci.,* 2005, **262**, 436–444.