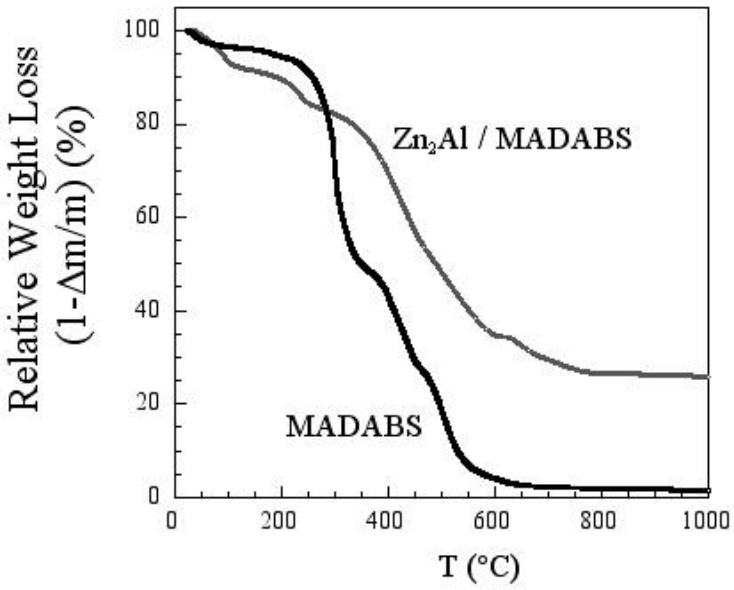

Fig. SEI-1

TG analysis of MADABS and Zn_2Al/MADAS performed under air with a heating slope of 5°C/min.

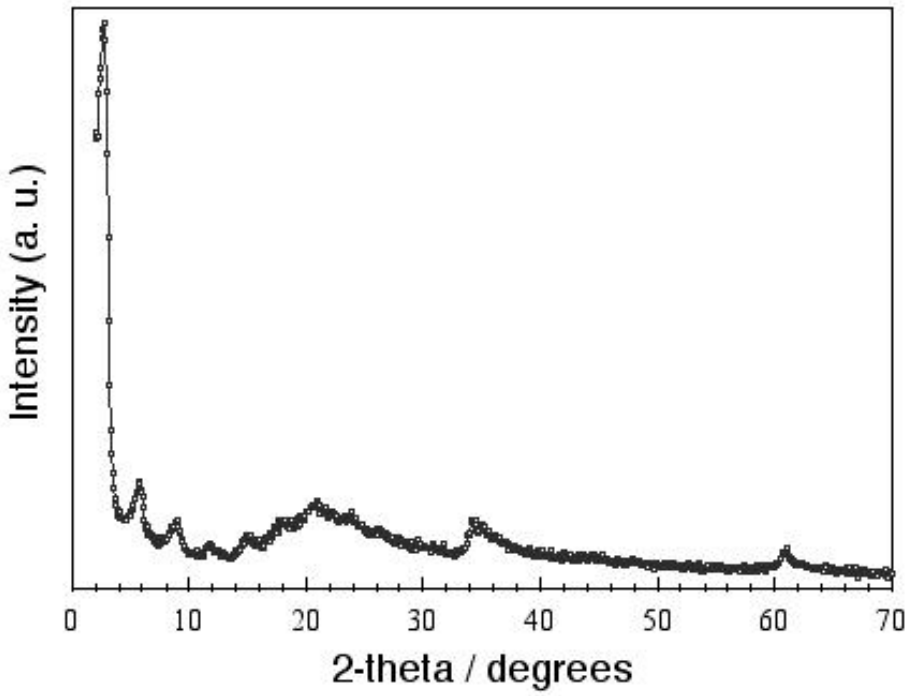

Fig. SEI - 2. XRD of Zn_2Al/MADABS-200°C

^{13}C (I = 1/2) solid state NMR experiments were performed with a 300 Bruker spectrometer at 75.47 MHz, using magic angle spinning (MAS) condition at 10 kHz and a 4 mm diameter size zirconia rotor. ^{13}C spectra obtained by proton enhanced cross-polarization method (CP) were referenced to the carbonyl of the glycine calibrated at 176.03 ppm.

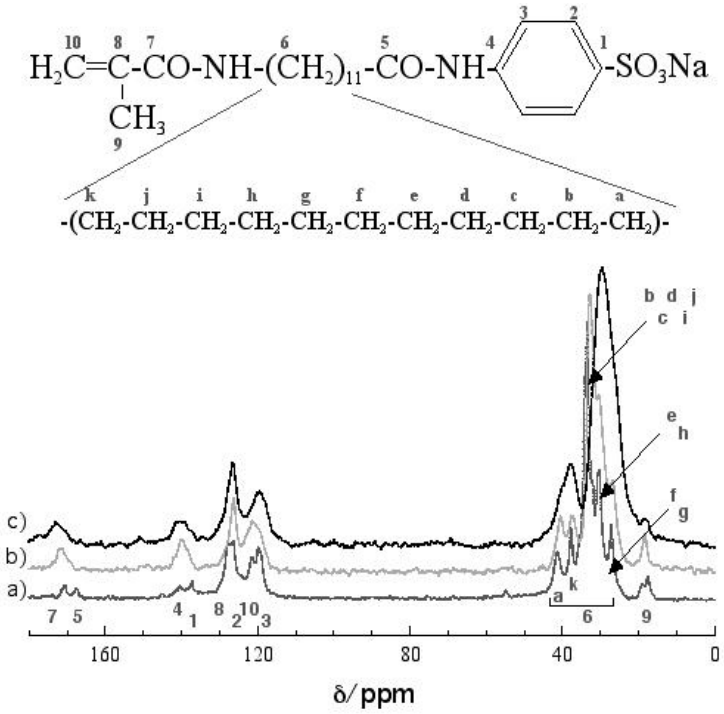

Fig. SEI – 3

^{13}CP-MAS NMR on a) MADABS, b) Zn_2Al/MADABS and c) Zn_2Al/MADABS-200

DSC The differential scanning calorimeter used to measure the glass transition T_g was a Mettler Toledo DSC30. The heating rate was 10°C per minute and the temperature range was from 25 to 180°C, Tg was measured at the second heating step.

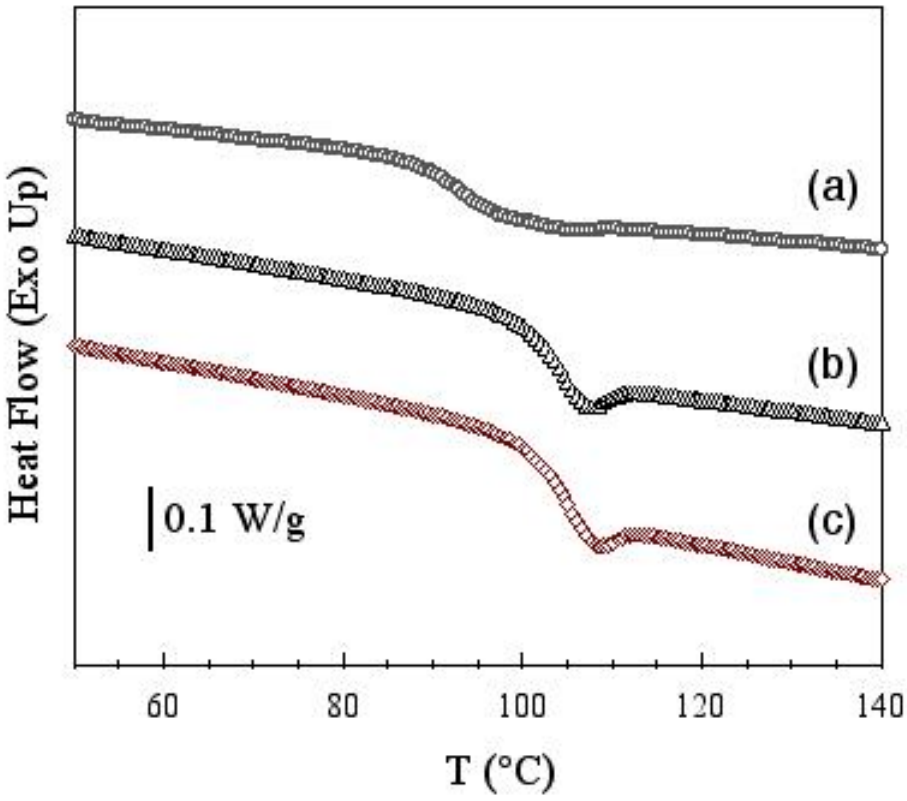

Fig. SEI-4

Glass transition temperature Tg of a) PS and PS nanocomposite derivatives in which the filler was calcined at 200°C c) or not b) before its dispersion into PS.

SEI-5

Molecular simulation of MADABS

SUMMARY OF PM6 CALCULATION

MOPAC2007 (Version: 7.323W)
Empirical Formula: C22 H33 N2 O5 S

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -132.45844 KCAL = -554.20612 KJ
TOTAL ENERGY = -5131.75752 EV
ELECTRONIC ENERGY = -39339.38987 EV
CORE-CORE REPULSION = 34207.63235 EV
DIPOLE = 8.84558 DEBYE POINT GROUP: C1
NO. OF FILLED LEVELS = 0
IONIZATION POTENTIAL = 9.357877 EV
MOLECULAR WEIGHT = 437.573

MOLECULAR DIMENSIONS (Angstroms)

Atom		Atom		Distance
O	28	H	33	21.86700
H	57	O	30	9.05092
H	60	H	56	4.11666

SCF CALCULATIONS = 137
COMPUTATION TIME = 1 MINUTES AND 1.578 SECONDS

C	0.00000000 +0	0.0000000 +0	0.0000000 +0				-0.2997
C	1.42872805 +1	0.0000000 +0	0.0000000 +0	1	0	0	-0.1150
C	1.47239460 +1	122.1827537 +1	0.0000000 +0	2	1	0	-0.4437
C	1.49168347 +1	118.3973903 +1	176.3233910 +1	2	1	3	0.5910
O	1.21898292 +1	124.1926932 +1	-77.6959160 +1	4	2	1	-0.5314
N	1.40008284 +1	114.1169673 +1	105.0174291 +1	4	2	1	-0.5101
C	1.48258184 +1	120.6770586 +1	-173.9993381 +1	6	4	2	-0.0896
C	1.53725156 +1	111.5244862 +1	103.6908249 +1	7	6	4	-0.3071
C	1.53332499 +1	110.7766190 +1	178.8962205 +1	8	7	6	-0.2552
C	1.53460561 +1	111.3380650 +1	179.9934748 +1	9	8	7	-0.2619
C	1.53441030 +1	111.3533422 +1	-178.7386434 +1	10	9	8	-0.2632
C	1.53452996 +1	111.3931675 +1	-178.8020290 +1	11	10	9	-0.2624
C	1.53456279 +1	111.3992854 +1	-179.2372226 +1	12	11	10	-0.2630
C	1.53438079 +1	111.3480277 +1	-178.2549576 +1	13	12	11	-0.2606
C	1.53530640 +1	111.4058956 +1	179.6237816 +1	14	13	12	-0.2729
C	1.53315009 +1	111.0669923 +1	-176.7026468 +1	15	14	13	-0.2272
C	1.53427071 +1	112.9810274 +1	-174.7311057 +1	16	15	14	-0.4213
C	1.51401113 +1	110.9670917 +1	-71.8103889 +1	17	16	15	0.6305
O	1.20994493 +1	124.3300083 +1	-83.5966849 +1	18	17	16	-0.4917

N	1.42887927 +1	113.9425688 +1	97.1309680 +1	18	17	16	-0.5216
C	1.41829044 +1	126.4117934 +1	-179.6747084 +1	20	18	17	0.3783
C	1.41793264 +1	117.3157455 +1	177.3727794 +1	21	20	18	-0.4065
C	1.38890059 +1	119.4774901 +1	179.6835055 +1	22	21	20	0.1395
C	1.40285675 +1	120.5843693 +1	0.0458483 +1	23	22	21	-0.7125
C	1.40336627 +1	119.6861996 +1	-0.3455511 +1	24	23	22	0.1328
C	1.41010213 +1	122.6425545 +1	-3.1608374 +1	21	20	18	-0.3669
S	1.71168081 +1	119.9442024 +1	-179.6225679 +1	24	23	22	2.4032
O	1.43881808 +1	112.0570443 +1	159.3561027 +1	27	24	23	-0.8880
O	1.44060634 +1	111.8760677 +1	20.5446275 +1	27	24	23	-0.8933
O	1.68651039 +1	95.3681070 +1	-89.6443944 +1	27	24	23	-0.4128
H	1.07049114 +1	121.3762280 +1	89.0168336 +1	1	2	3	0.1572
H	1.07366677 +1	120.4039851 +1	-90.8484439 +1	1	2	3	0.1687
H	1.10119977 +1	111.8425307 +1	29.4554528 +1	3	2	1	0.1701
H	1.10145333 +1	112.2849775 +1	150.0260752 +1	3	2	1	0.1713
H	1.10238137 +1	110.7828594 +1	-89.9670558 +1	3	2	1	0.1676
H	1.01354567 +1	120.6319154 +1	-11.6630781 +1	6	4	2	0.2668
H	1.11222780 +1	108.3036277 +1	-134.0419370 +1	7	6	4	0.1322
H	1.11832257 +1	108.8242561 +1	-18.1099501 +1	7	6	4	0.1663
H	1.10877898 +1	109.6009160 +1	-59.5409304 +1	8	7	6	0.1503
H	1.10632231 +1	110.4525102 +1	56.7151552 +1	8	7	6	0.1357
H	1.10734393 +1	110.0725396 +1	-57.9289188 +1	9	8	7	0.1320
H	1.10831660 +1	109.8159100 +1	58.2309009 +1	9	8	7	0.1377
H	1.10755589 +1	109.8653446 +1	-56.7575495 +1	10	9	8	0.1347
H	1.10721907 +1	109.8807723 +1	59.2592163 +1	10	9	8	0.1320
H	1.10731163 +1	109.9128834 +1	-56.7638176 +1	11	10	9	0.1329
H	1.10738460 +1	109.8337609 +1	59.2232737 +1	11	10	9	0.1335
H	1.10728938 +1	109.8816424 +1	-57.1588266 +1	12	11	10	0.1331
H	1.10749138 +1	109.7800077 +1	58.7808788 +1	12	11	10	0.1333
H	1.10759326 +1	109.7674547 +1	-56.3125547 +1	13	12	11	0.1339
H	1.10705447 +1	109.8208819 +1	59.6636438 +1	13	12	11	0.1319
H	1.10733095 +1	109.8768435 +1	-58.2151964 +1	14	13	12	0.1342
H	1.10806131 +1	109.7093663 +1	57.6778572 +1	14	13	12	0.1370
H	1.10779642 +1	109.4943910 +1	-54.9323019 +1	15	14	13	0.1374
H	1.10673334 +1	109.5939425 +1	61.2351612 +1	15	14	13	0.1309
H	1.10954889 +1	109.8583879 +1	-53.3103835 +1	16	15	14	0.1439
H	1.11066826 +1	110.0133236 +1	62.3658288 +1	16	15	14	0.1513
H	1.11502636 +1	109.2438588 +1	169.7877666 +1	17	16	15	0.1903
H	1.10677310 +1	110.7875251 +1	54.4916731 +1	17	16	15	0.1705
H	1.02524100 +1	117.6032925 +1	-3.7718506 +1	20	18	17	0.2805
H	1.08751453 +1	120.8187968 +1	-0.1457360 +1	22	21	20	0.1766
H	1.09795436 +1	119.5617908 +1	-179.4876563 +1	23	22	21	0.1531
H	1.09824897 +1	119.8921220 +1	-179.2003824 +1	25	24	23	0.1564
H	1.09754756 +1	120.3206293 +1	0.4019725 +1	26	21	20	0.2191
