

Supplementary Information

Design of lamellar structured POSS/BPZ polybenzoxazine nanocomposites as the novel class of ultra low k dielectric material.

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Spectral data of 1,1-Bis(4-hydroxyphenyl)-cyclohexane (Bisphenol Z)

FT-IR (KBr, cm⁻¹): 3586 (free OH), 3240 (hydrogen bonded OH), 2931 (cyclohexyl symmetric stretching C-H bond), 2853 (cyclohexyl asymmetric stretching C-H bond), 819 (Para substituted benzene).

¹H NMR (400MHz, CDCl₃) δ (ppm): 8.25 (bs, 1H, OH), 6.72 (d, 4H, Ar), 7.05 (d, 4H, Ar), 2.17 (m, 4H, cyclohexyl), 1.52-1.46 (m, 6H, cyclohexyl).

Spectral data of bisphenol Z benzoxazine (BPZ-Bz)

FT-IR (KBr, cm⁻¹): 948 (N-C-O), 1232 (C-O-C), 1376 (CH₂ wagging) and 1508 (tri-substituted benzene ring).

¹H NMR (400MHz, CDCl₃) δ (ppm): 7.28-6.7 (m, 16H, Ar), 5.31 (s, 4H, O-CH₂-N), 4.58 (s, 4H, Ar-CH₂-N), 2.15-2.14 (m, 4H, cyclohexyl) and 1.51-1.49 (m, 6H, cyclohexyl).

Spectral data of 2-allyl phenol benzoxazine (AP-Bz)

FT-IR (KBr, cm⁻¹): 941 (N-O-C), 1221 (Ar-C-N), 3032 (allylic C-H), 1595 (allylic C=C stretching) and 754 (ortho-substituted benzene ring).

¹H NMR (400MHz, CDCl₃) δ (ppm): 7.28-6.82 (m, 8H, Ar), 6.00-5.93 (m, 1H, =CH), 5.37 (s, 2H, O-CH₂-N), 5.04-5.00 (s, 2H, =CH₂), 4.62 (s, 2H, Ar-CH₂-N) and 3.34-3.32 (allylic CH₂).

Spectral data of OHC-POSS

FT-IR (KBr, cm⁻¹): 2145 (Si-H stretching), 902 (Si-H bending), 1260 (Si-CH₃) and 1097 (Si-O-Si asymmetric stretching).

¹H NMR (400MHz, CDCl₃) δ (ppm): 4.74-4.72 (m, 1H, Si-H), and 0.26-0.25 (m, 6H, Si(CH₃)₂).

Spectral data of POSS-Bz

FT-IR (KBr, cm⁻¹): 1092 (Si-O-Si), 945 (N-O-C asymmetric stretching), 1222 (Ar-C-N asymmetric stretching of benzoxazine ring), 2145 (disappearance of Si-H) and 1166 (appearance of Si-CH₂-CH₂).

¹H NMR (400MHz, CDCl₃) δ (ppm): 7.24-6.76 (m, 8H, Ar), 5.28 (s, 2H, O-CH₂-N), 4.56 (s, 2H, Ar-CH₂-N), 2.58-2.54 (m, 2H, Ar-CH₂), 1.59-1.57 (m, 2H, Si-CH₂-CH₂), 0.65-0.61 (m, 2H, Si-CH₂) and 0.09 [Si-(CH₃)₂].

²⁹Si NMR (500MHz, CDCl₃) δ (ppm): 18.78 [Si-(CH₃)₂] and -102.95 (Si-O-Si).

¹³C NMR (400MHz, CDCl₃) δ (ppm): 152.2 (Ar-C), 148.5 (Ar-C), 130.5 (Ar-C), 129.2 (Ar-CH), 128.3 (Ar-CH), 124.2 (Ar-CH), 121.1 (Ar-CH), 120.29 (Ar-C), 120.2 (Ar-CH), 118.0 (Ar-CH), 79.0 (O-CH₂-N), 50.7 (Ar-CH₂-N), 33.1 (Ar-CH₂-CH₂), 23.3 (Si-CH₂-CH₂), 17.6 (Si-CH₂).

DEPT-135 NMR (400MHz, CDCl₃) δ (ppm): 129.2 (Ar-CH), 128.3 (Ar-CH), 124.2 (Ar-CH), 121.1 (Ar-CH), 120.2 (Ar-CH), 118.0 (Ar-CH) (down-field region regarding CH and CH₃), 79.0 (O-CH₂-N), 50.7 (Ar-CH₂-N), 33.1 (Ar-CH₂-CH₂), 23.3 (Si-CH₂-CH₂), 17.6 (Si-CH₂) (up-field region regarding CH₂).