

Supplementary Materials

Side group topological structure modified orbital and condensed state characteristics enhance the electrical anti-breakdown performance of polyolefin

Shixun Hu^{1*}, Cheng Tong¹, Xiongjie Yang¹, Shangshi Huang¹, Jun Hu¹, Qi Li^{1*},
Jinliang He^{1*}

1) Department of Electrical Engineering, Tsinghua University, Beijing, 100084, China.

***Corresponding author:** Jinliang He, hejl@tsinghua.edu.cn; Qi Li, qili1020@tsinghua.edu.cn; Shixun Hu, rugals@yeah.net

Detailed data of MD analysis

1. Free volume region distribution in real space

PP-g-VAc-A
@ 30 °C

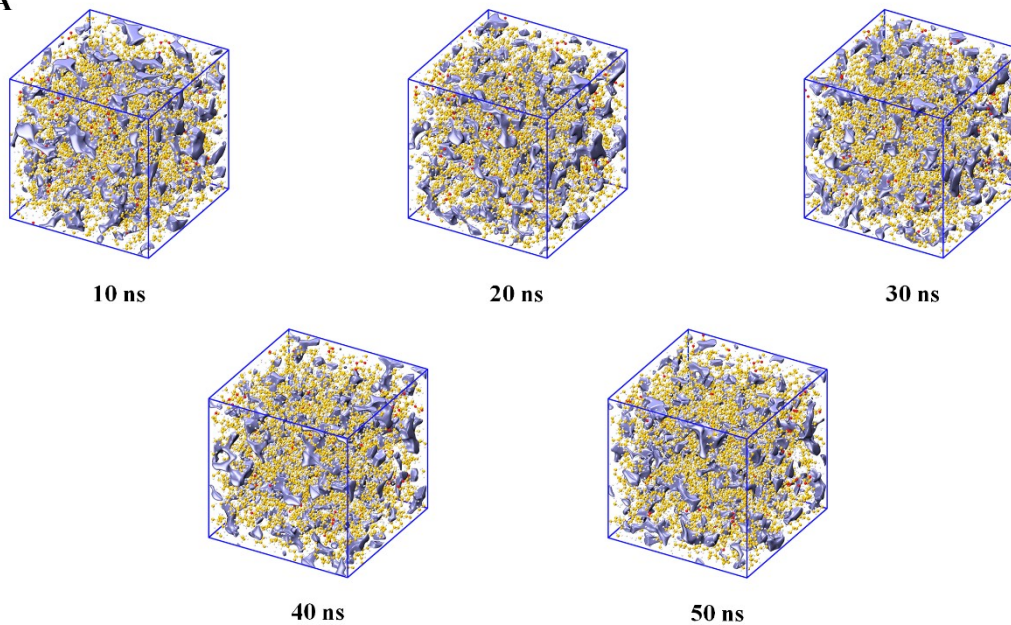


Figure S1 Free volume region distribution of PP-g-VAc-A system at different moments under 30 °C.

PP-g-VAc-B
@ 30 °C

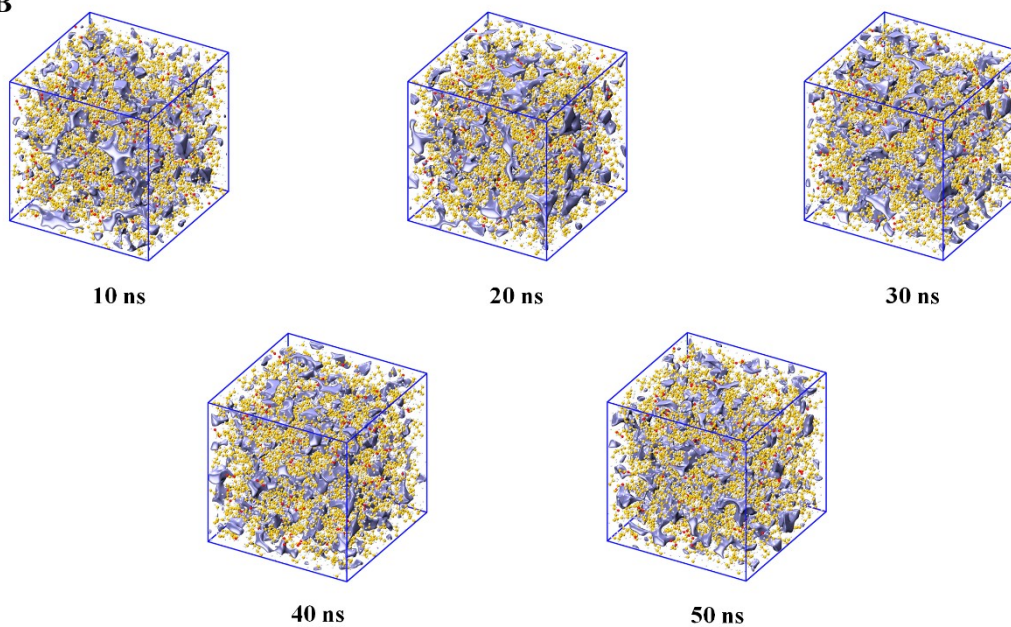


Figure S2 Free volume region distribution of PP-g-VAc-B system at different moments under 30 °C.

PP-g-NVP-A
@ 30 °C

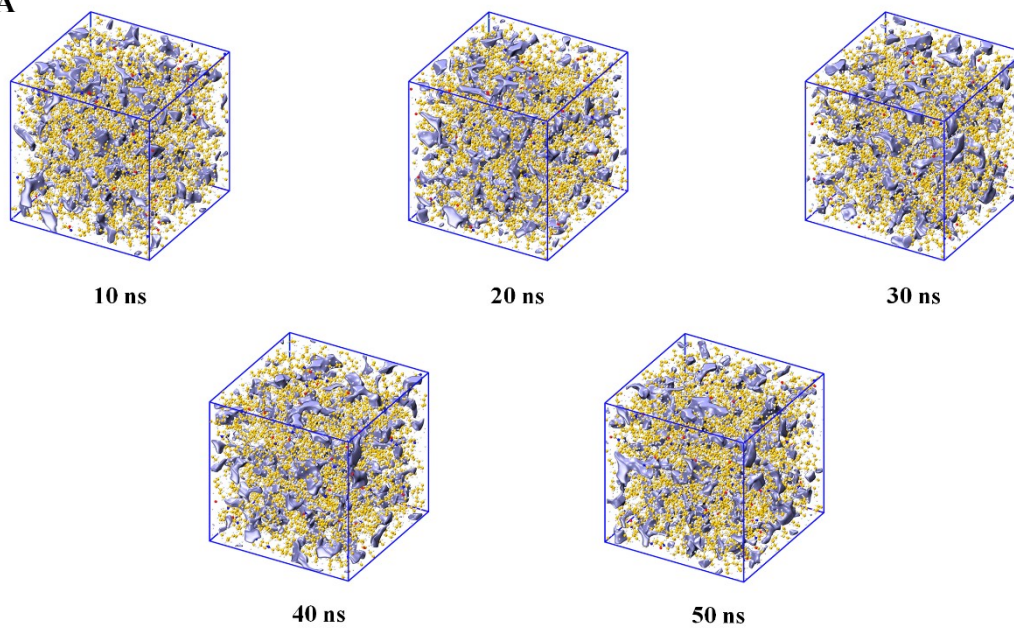


Figure S3 Free volume region distribution of PP-g-NVP-A system at different moments under 30 °C.

PP-g-NVP-B
@ 30 °C

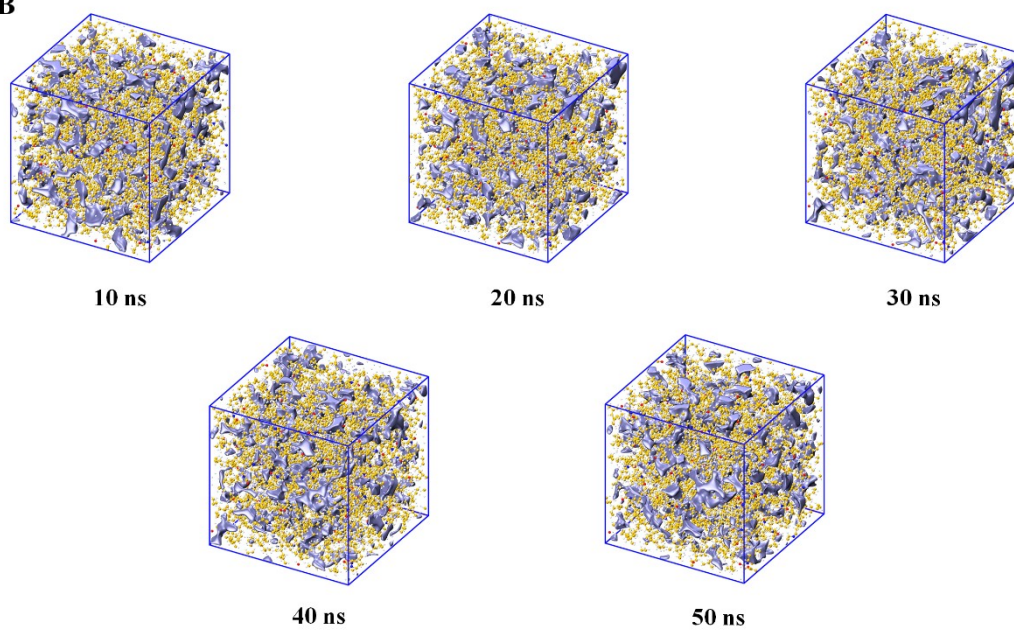


Figure S4 Free volume region distribution of PP-g-NVP-B system at different moments under 30 °C.

PP-g-VAc-A
@ 90 °C

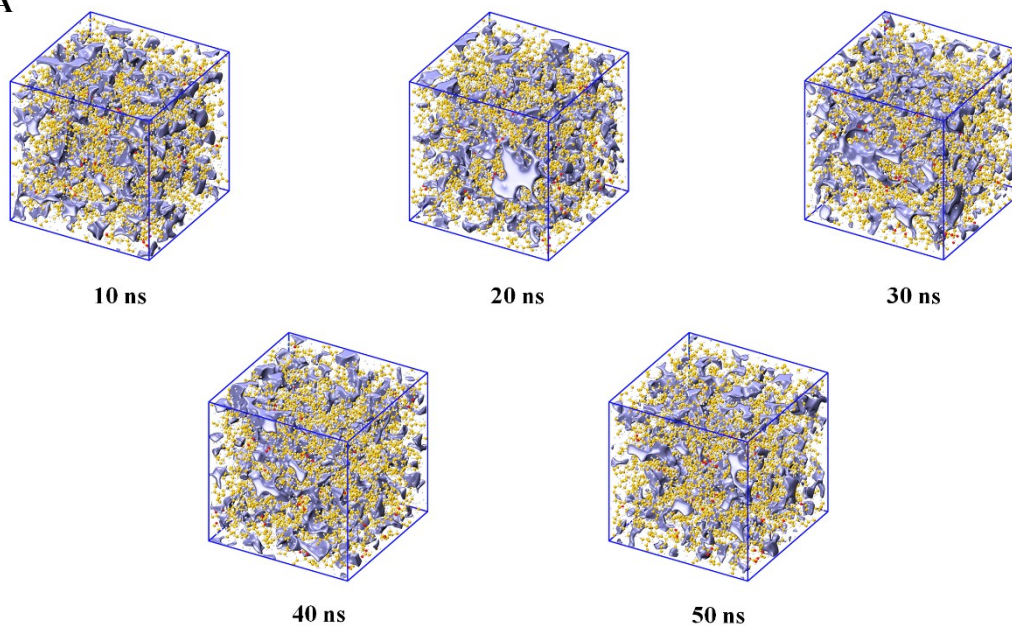


Figure S5 Free volume region distribution of PP-g-VAc-A system at different moments under 90 °C.

PP-g-VAc-B
@ 90 °C

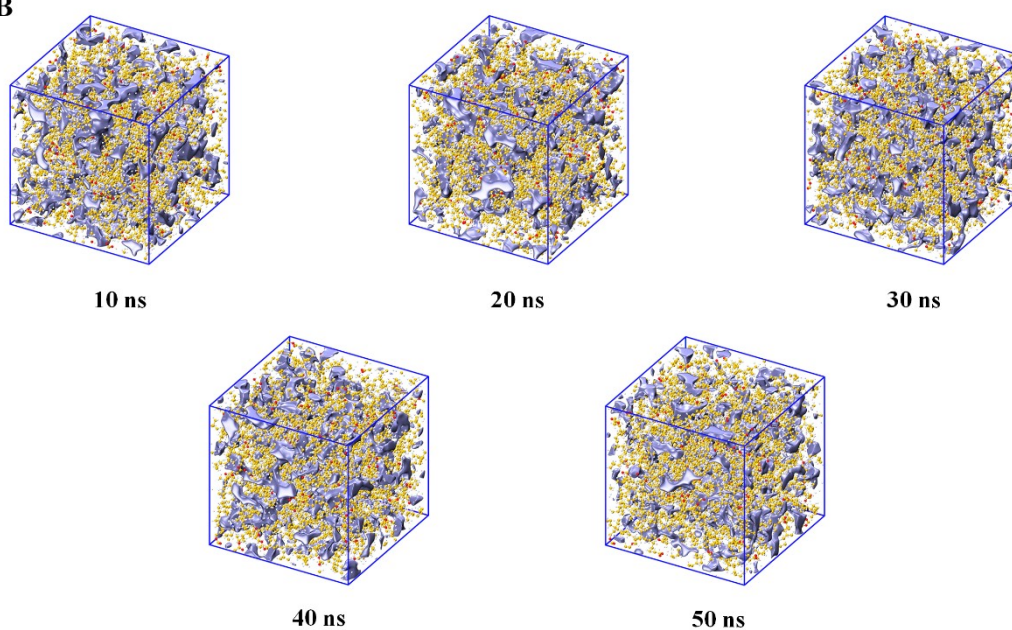


Figure S6 Free volume region distribution of PP-g-VAc-B system at different moments under 90 °C.

PP-g-NVP-A
@ 90 °C

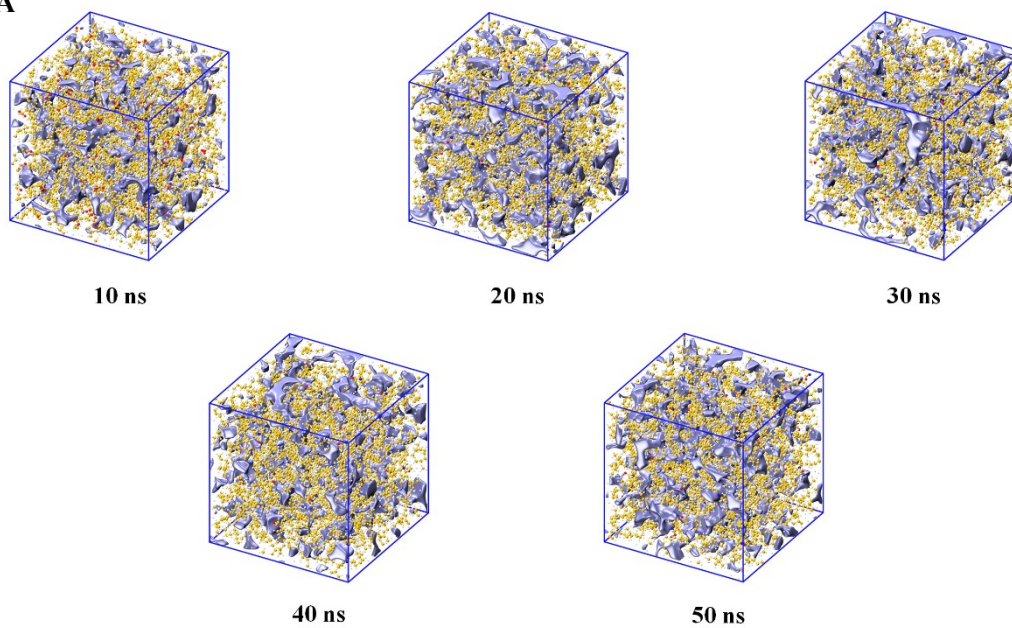


Figure S7 Free volume region distribution of PP-g-NVP-A system at different moments under 90 °C.

PP-g-NVP-B
@ 90 °C

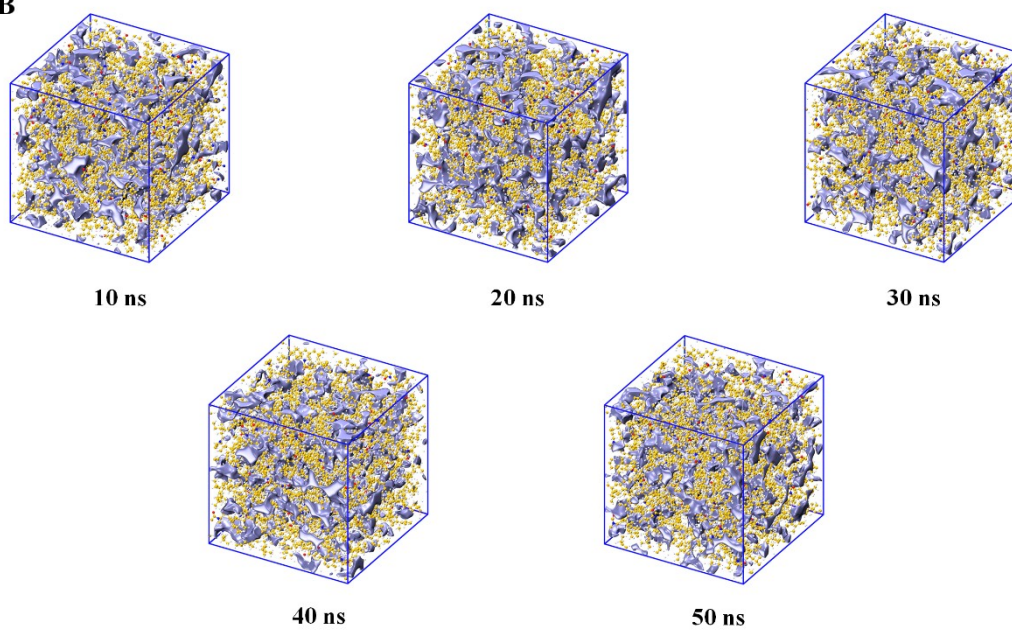


Figure S8 Free volume region distribution of PP-g-NVP-B system at different moments under 90 °C.

2. Statistical free volume parameters

Table SI Statistical free volume parameters of PP-g-VAc-A under 30 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-VAc-A-10ns	90.91	36.02	39.62
PP-g-VAc-A-20ns	90.23	35.34	39.16
PP-g-VAc-A-30ns	89.95	35.06	38.98
PP-g-VAc-A-40ns	90.01	35.11	39.01
PP-g-VAc-A-50ns	90.13	35.24	39.10
Average value	90.25	35.35	39.17
Standard deviation	0.35	0.35	0.23

Table SII Statistical free volume parameters of PP-g-VAc-B under 30 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-VAc-B-10ns	96.26	37.40	38.85
PP-g-VAc-B-20ns	96.53	37.70	39.05
PP-g-VAc-B-30ns	95.89	37.05	38.64
PP-g-VAc-B-40ns	96.29	37.46	38.90
PP-g-VAc-B-50ns	95.81	36.97	38.58
Average value	96.16	37.31	38.80
Standard deviation	0.27	0.27	0.17

Table SIII Statistical free volume parameters of PP-g-NVP-A under 30 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-NVP-A-10ns	91.91	35.63	38.77
PP-g-NVP-A-20ns	92.05	35.79	38.88
PP-g-NVP-A-30ns	92.45	36.18	39.13
PP-g-NVP-A-40ns	92.24	35.96	38.98
PP-g-NVP-A-50ns	91.79	35.51	38.69
Average value	92.09	35.81	38.89
Standard deviation	0.24	0.24	0.16

Table SIV Statistical free volume parameters of PP-g-NVP-B under 30 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-NVP-B-10ns	100.40	38.84	38.68
PP-g-NVP-B-20ns	99.88	38.35	38.40
PP-g-NVP-B-30ns	100.37	38.83	38.69
PP-g-NVP-B-40ns	100.60	39.03	38.80

PP-g-NVP-B-50ns	100.50	38.97	38.77
Average value	100.35	38.80	38.67
Standard deviation	0.25	0.24	0.14

Table SV Statistical free volume parameters of PP-g-VAc-A under 90 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-VAc-A-10ns	93.84	38.95	41.50
PP-g-VAc-A-20ns	92.92	38.05	40.95
PP-g-VAc-A-30ns	92.99	38.09	40.96
PP-g-VAc-A-40ns	93.04	38.13	40.98
PP-g-VAc-A-50ns	92.56	37.68	40.71
Average value	93.07	38.18	41.02
Standard deviation	0.42	0.42	0.26

Table SVI Statistical free volume parameters of PP-g-VAc-B under 90 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-VAc-B-10ns	98.61	39.78	40.34
PP-g-VAc-B-20ns	99.05	40.22	40.60
PP-g-VAc-B-30ns	98.86	40.00	40.46
PP-g-VAc-B-40ns	99.03	40.18	40.57
PP-g-VAc-B-50ns	97.77	38.90	39.79
Average value	98.67	39.82	40.35
Standard deviation	0.47	0.48	0.30

Table SVII Statistical free volume parameters of PP-g-NVP-A under 90 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-NVP-A-10ns	94.69	38.44	40.60
PP-g-NVP-A-20ns	95.06	38.79	40.80
PP-g-NVP-A-30ns	94.66	38.37	40.53
PP-g-NVP-A-40ns	93.91	37.65	40.09
PP-g-NVP-A-50ns	94.41	38.16	40.42
Average value	94.54	38.28	40.49
Standard deviation	0.38	0.38	0.23

Table SVIII Statistical free volume parameters of PP-g-NVP-B under 90 °C

Designation	Box volume (nm ³)	Free volume (nm ³)	Free volume proportion (%)
PP-g-NVP-B-10ns	103.13	41.58	40.32
PP-g-NVP-B-20ns	103.34	41.81	40.46

PP-g-NVP-B-30ns	101.90	40.38	39.63
PP-g-NVP-B-40ns	102.04	40.49	39.68
PP-g-NVP-B-50ns	101.97	40.45	39.67
Average value	102.48	40.95	39.95
Standard deviation	0.62	0.62	0.36

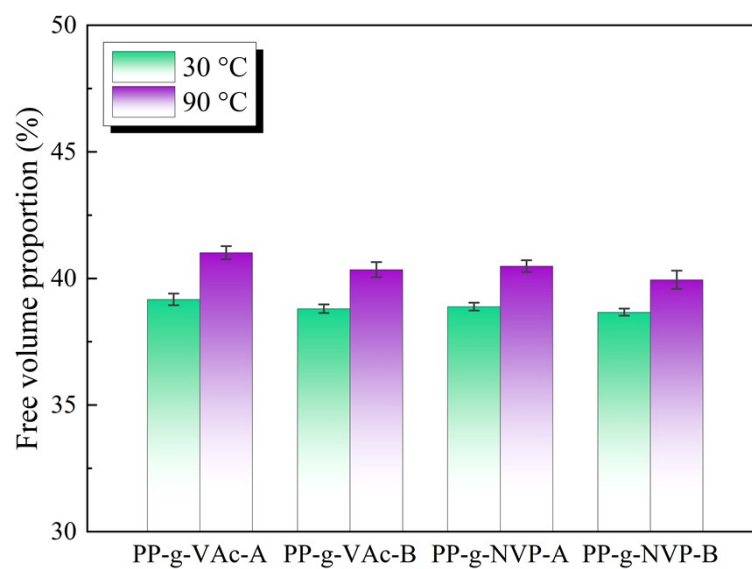


Figure S9 Free volume proportion of different MD systems under 30 and 90 °C.