Supporting Information: Computable Bulk and Interfacial Electronic Structure Features as Proxies for Dielectric Breakdown of Polymers

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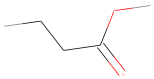
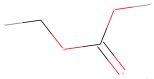
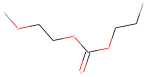
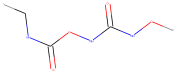
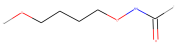
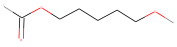
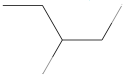
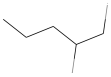
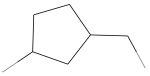
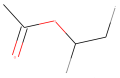
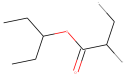
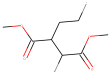
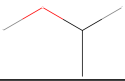
1 Potential high breakdown polymers

No.	Polymer name	Repeat unit	E_{gap}	ϕ_e	ϕ_h	Ref.
1	poly(1-ethylene)		6.70	3.42	3.28	
2			6.91	3.21	3.70	
3			7.82	3.13	4.70	
4			6.56	3.26	3.29	
5			6.55	3.09	3.46	
6			6.79	3.31	3.48	
7			7.19	3.46	3.73	
8			8.88	3.31	5.57	
9			8.01	3.18	4.83	
10			7.97	3.31	4.65	
11	poly(1-ethylethylene)		6.32	3.27	3.05	1
12	poly(1-propylethylene)		6.53	3.38	3.15	2
13	poly(cyclopentane-1,3-diylmethylene)		6.73	3.36	3.37	3
14	poly[1-(acetyloxy)ethylene]		6.65	3.21	3.44	4
15	poly[1-[1-(ethylpropoxy)carbonyl]ethylene]		6.24	3.22	3.02	5
16	poly[1,2-bis(methoxycarbonyl)butane-1,4-diyl]		6.40	3.24	3.16	6
17	poly[oxy(methylmethylene)]		6.73	3.40	3.33	7

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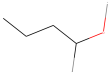
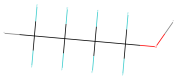
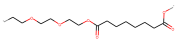
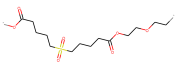
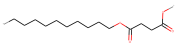
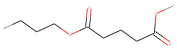
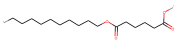
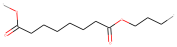
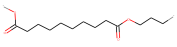
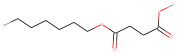
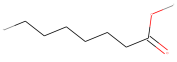
No.	Polymer name	Repeat unit	E_{gap}	ϕ_e	ϕ_h	Ref.
18	poly[oxy(propylmethylene)]		6.46	3.29	3.17	8
19	poly[oxy(1,1,2,2,3,3,4,4-octafluorobutane-1,4-diyl)]		8.89	3.02	5.87	9
20	poly(oxyethyleneoxyethylene-oxyethyleneoxyoctanedioyl)		6.47	3.15	3.31	10
21	poly[oxyethyleneoxyethyl-eneoxy(1-oxopentane-1,5-diyl)sulfonyl(5-oxopentane-1,5-diyl)]		6.34	3.10	3.24	11
22	poly(oxybutanedioyloxydecane-1,10-diyl)		6.52	3.17	3.35	12
23	poly(oxypropane-1,3-diyloxypentanedioyl)		6.53	3.12	3.41	13
24	poly(oxyhexanedioyloxydecane-1,10-diyl)		6.33	3.16	3.18	14
25	poly(oxypropane-1,3-diyloxyoctanedioyl)		6.71	3.36	3.35	15
26	poly(oxypropane-1,3-diyloxydecanedioyl)		6.64	3.39	3.25	16
27	poly(oxybutanedioyloxyhexane-1,6-diyl)		6.41	3.12	3.29	17
28	poly[oxy(1-oxoheptane-1,7-diyl)]		6.27	3.11	3.16	18

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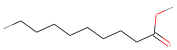
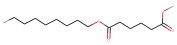
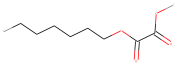
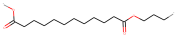
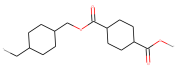
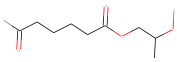
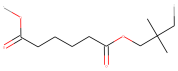
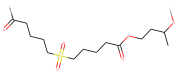
No.	Polymer name	Repeat unit	E_{gap}	ϕ_e	ϕ_h	Ref.
29	poly[oxy(1-oxononane-1,9-diyl)]		6.25	3.16	3.09	19
30	poly(oxyhexanedioyloxyoctane-1,8-diyl)		6.56	3.34	3.21	14
31	poly(oxyethanedioyloxyhexane-1,6-diyl)		6.81	3.48	3.33	20
32	poly[oxy(2-methyl-1-oxopropane-1,3-diyl)]		6.44	3.17	3.28	21
33	poly(oxypropane-1,3-diyloxydodecanedioyl)		6.32	3.18	3.14	22
34	poly(oxycarbonylcyclohexane-1,4-diylcarbonyloxymethylene-cyclohexane-1,4-diylmethylene)		6.38	3.11	3.27	23
35	poly[oxy(1-methylethylene)oxyhexanedioyl]		6.40	3.11	3.29	24
36	poly[oxy(2,2-dimethylpropane-1,3-diyl)oxyhexanedioyl]		6.47	3.25	3.22	25
37	poly[oxy(1-methylpropane-1,3-diyl)oxy(1-oxopentane-1,5-diyl)sulfonyl(5-oxopentane-1,5-diyl)]		6.54	3.29	3.25	26

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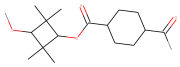
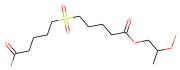
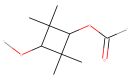
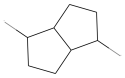
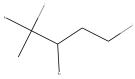
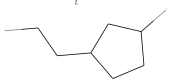
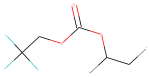
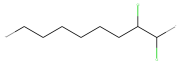
No.	Polymer name	Repeat unit	E_{gap}	ϕ_e	ϕ_h	Ref.
38	poly[oxy(2,2,4,4-tetramethylcyclobutane-1,3-diyl)oxycarbonylcyclohexane-1,4-diylcarbonyl]		6.29	3.07	3.22	27
39	poly[oxy(1-methylethylene)oxy(1-oxopentane-1,5-diyl)sulfonyl(5-oxopentane-1,5-diyl)]		6.48	3.02	3.46	26
40	poly[oxycarbonyloxy(2,2,4,4-tetramethylcyclobutane-1,3-diyl)]		6.30	3.24	3.06	28
41	poly(bicyclo[3.3.0]octane-2,6-diyl)		6.49	3.45	3.04	29
42	NaN		6.60	3.36	3.25	30
43	poly(cyclopentane-1,3-diylethylene)		6.96	3.49	3.46	31
44	poly[1-(2,2,2-trifluoroethoxy- carbony-loxy)ethylene]		7.31	3.01	4.30	32
45	poly(1,2-dichlorooctane-1,8-diyl)		6.65	3.19	3.46	33

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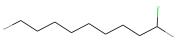
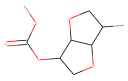
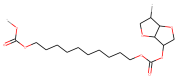
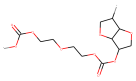
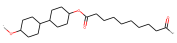
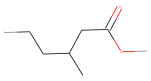
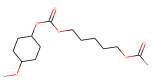
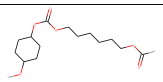
No.	Polymer name	Repeat unit	E_{gap}	ϕ_e	ϕ_h	Ref.
46	poly(1-chlorononane-1,9-diyl)		6.75	3.29	3.46	34
47	poly[(2,3,3a,5,6,6a-hexahydrofuro[3,2-b]furan-3,6-diyl)oxycarbonyloxy]		6.68	3.38	3.30	35
48	poly[(2,6-dioxabicyclo[3.3.0]octane-4,8-diyl)oxycarbonyloxydecane-1,10-diyloxycarbonyloxy]		6.55	3.44	3.11	36
49	poly[(2,6-dioxabicyclo[3.3.0]octane-4,8-diyl) oxycarbonyloxyethyleneoxy-ethyleneoxycarbonyloxy]		6.53	3.22	3.31	36
50	poly(oxy-1,1'-bicyclohexane-4,4'-diyloxydecanedioyl)		6.13	3.05	3.08	37
51	poly[oxy(3-methyl-1-oxopentane-1,5-diyl)]		6.61	3.33	3.28	38
52	poly(oxycarbonyloxy-cyclohexane-1,4-diyloxycarbonyloxypentane-1,5-diyl)		6.89	3.35	3.54	39

Continued on next page

No.	Polymer name	Repeat unit	E_{gap}	ϕ_e	ϕ_h	Ref.
53	poly(oxycarbonyloxy-cyclohexane-1,4-diyloxycarbonyloxyhexane-1,6-diyl)		7.05	3.59	3.46	39

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