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Supplementary

Strategic Development of Dielectric Strength Prediction Protocol for Perfluorocarbon and Nonperfluorocarbon Compounds

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Abstract: Predicting the dielectric strengths of organic compounds is critical for identifying potential insulating gases. However, experimental evaluation techniques are time-consuming, and current computational protocols are limited in scope. In this study, to develop a reliable prediction protocol for the dielectric strengths of a broad array of perfluorocarbon (PFC) and non-PFC compounds, systematic linear regression is combined with computational calculations of relevant core factors. The designed equation-based protocol is demonstrated to have four core factors, including two high-correlation factors (polarizability and molecular weight) and two critical factors (ionization energy and highest occupied molecular orbital (HOMO)–lowest unoccupied molecular orbital (LUMO) gap). The two critical factors are crucial for determining a suitable protocol, as reliable predictions of dielectric strength are only possible if the ionization energy and HOMO–LUMO gap are maintained within specified ranges for all the compounds. These findings can act as design guidelines for future computational protocols to predict the insulating properties of PFC and non-PFC compounds.

Keywords: dielectric strength; insulating gas; computational protocol; organic compound; regression; density functional theory

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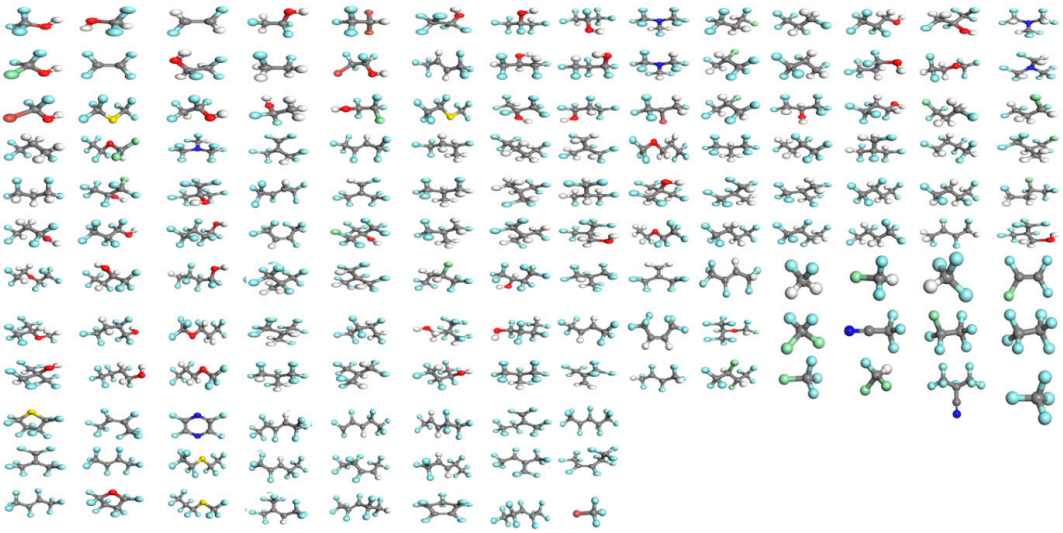


Figure S1. A total of 150 PFC compounds introduced in this study. Atoms with gray, white, red, blue, cyan, light green, and yellow in color depict carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine, and sulfur, respectively.

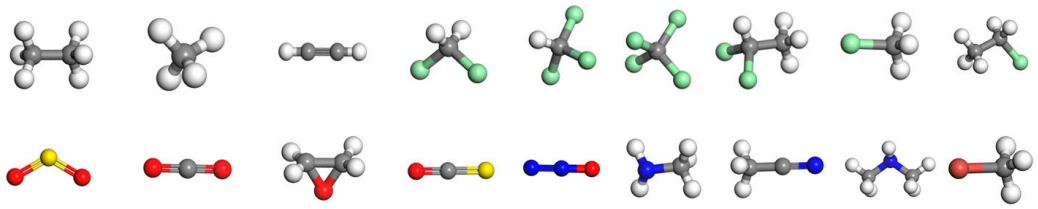
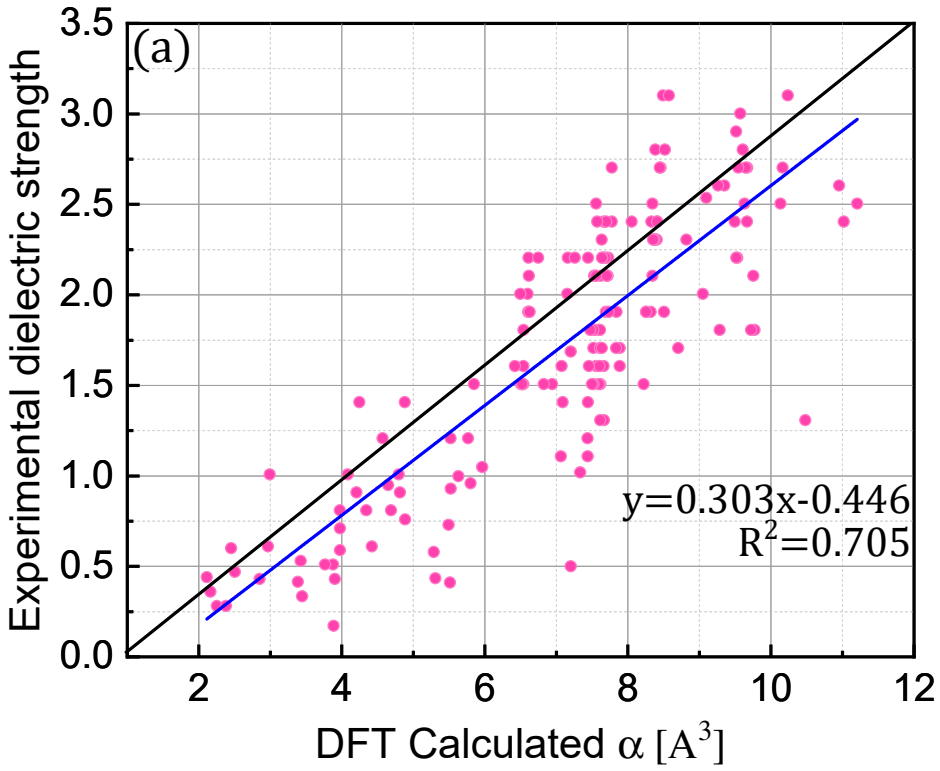
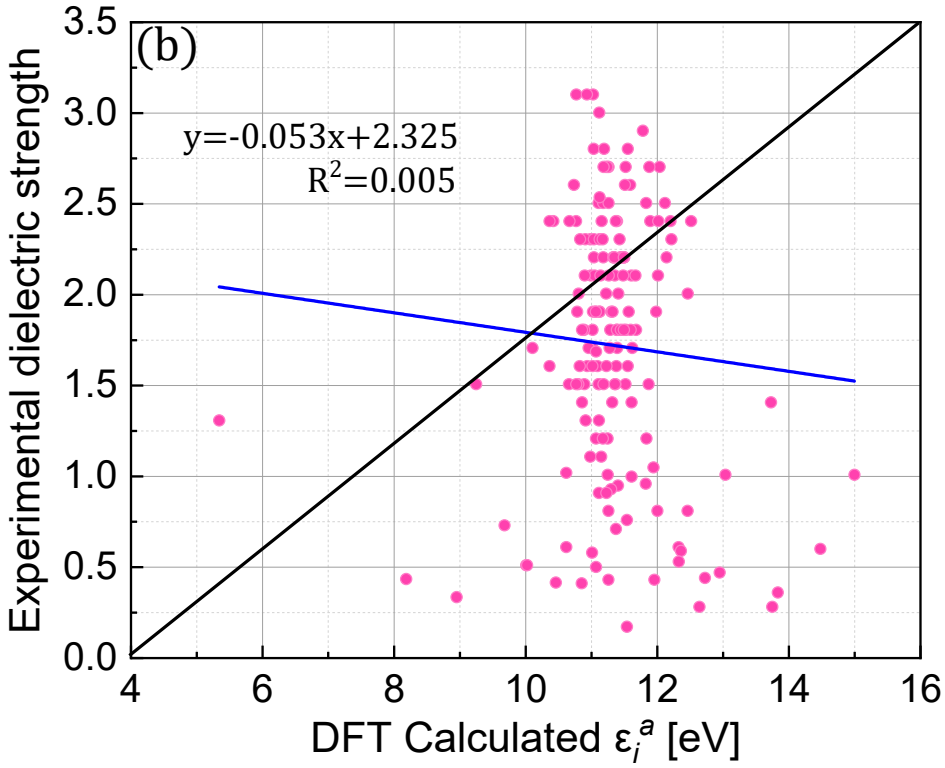
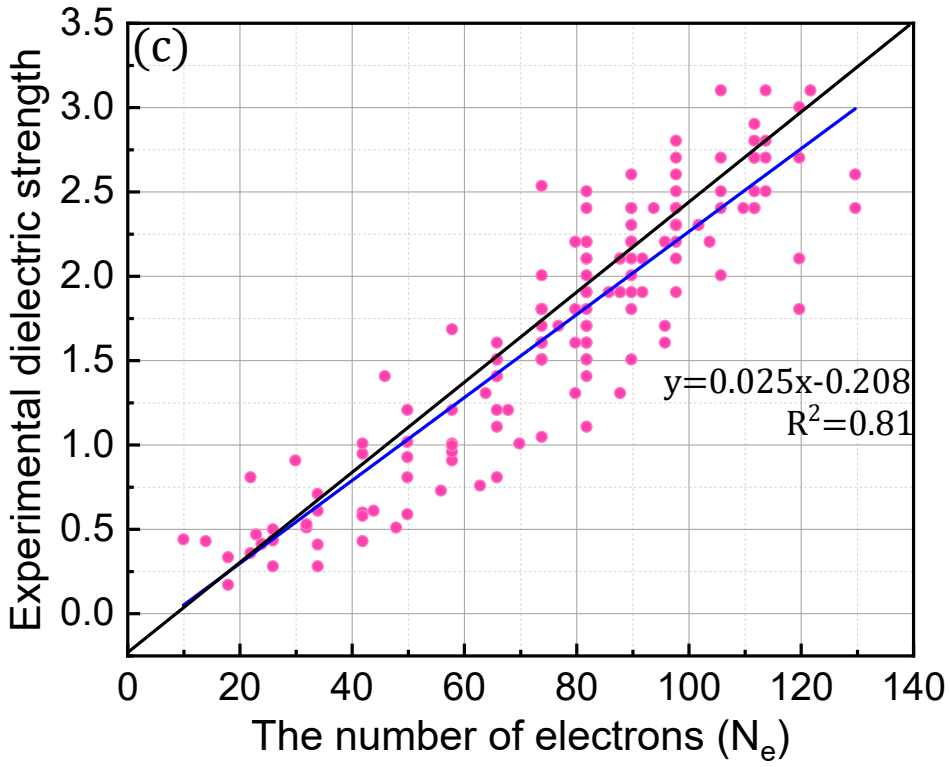
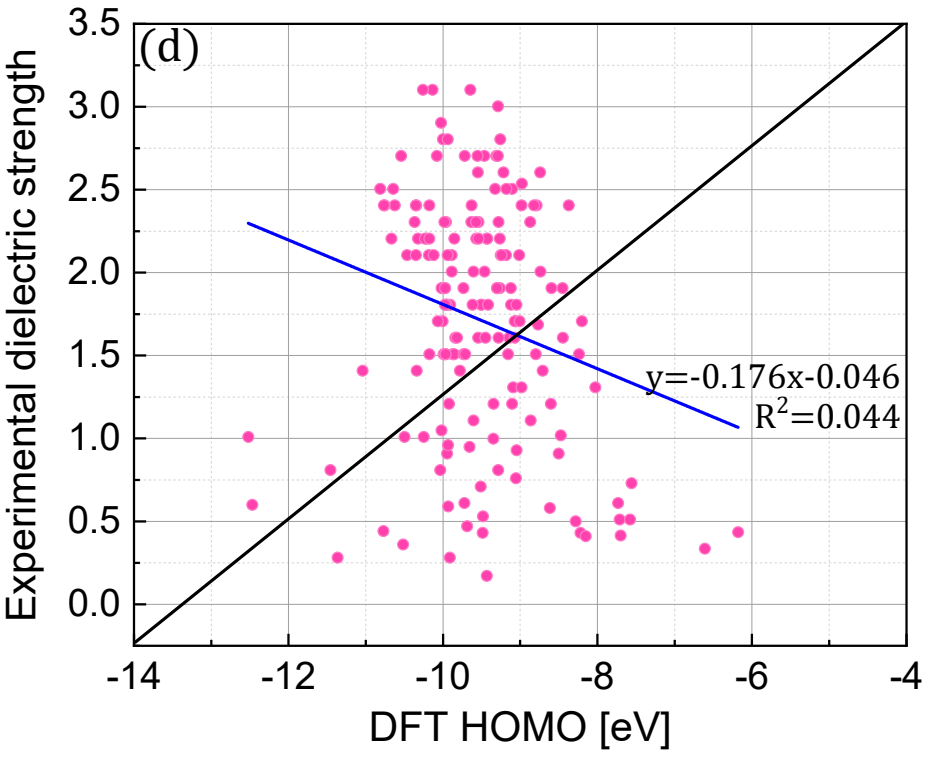


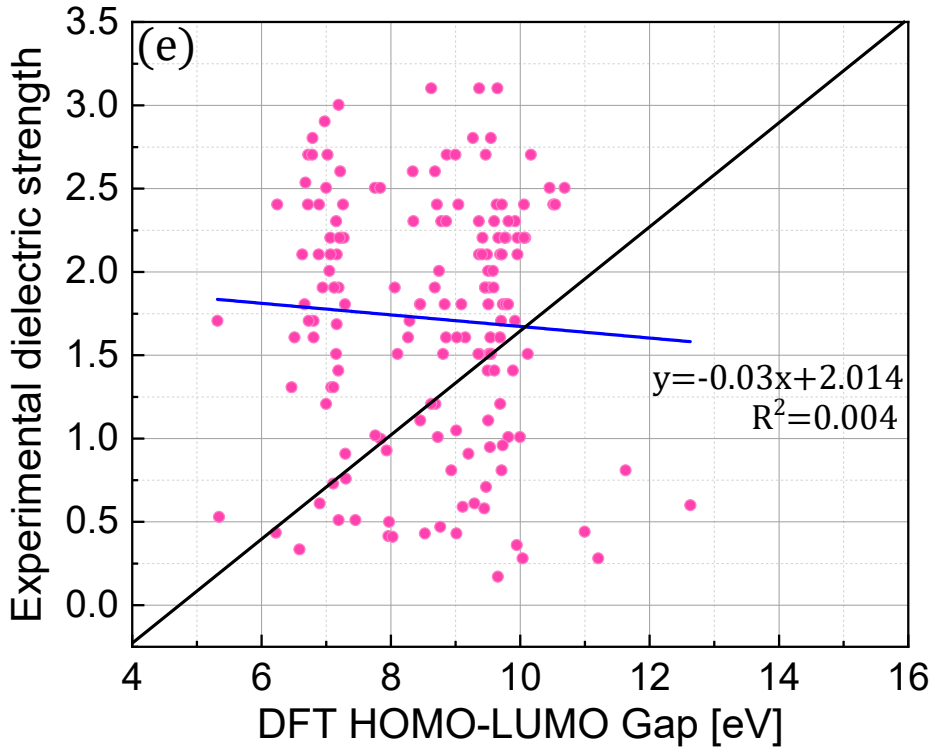
Figure S2. A total of 18 non-PFC compounds introduced in this study. Atoms with gray, white, red, blue, brown, light green, and yellow in color depict carbon, hydrogen, oxygen, nitrogen, bromine, chlorine, and sulfur, respectively.

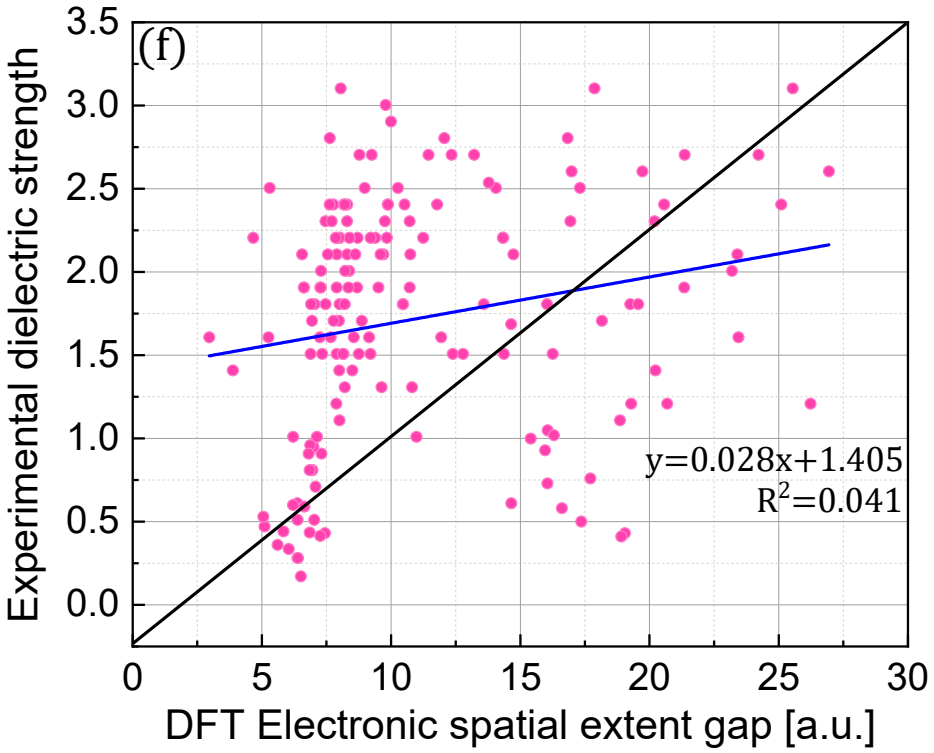

(a)
Experimental dielectric strength
DFT Calculated α [A^3]
y=0.303x-0.446
R^2=0.705
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
2
4
6
8
10
12

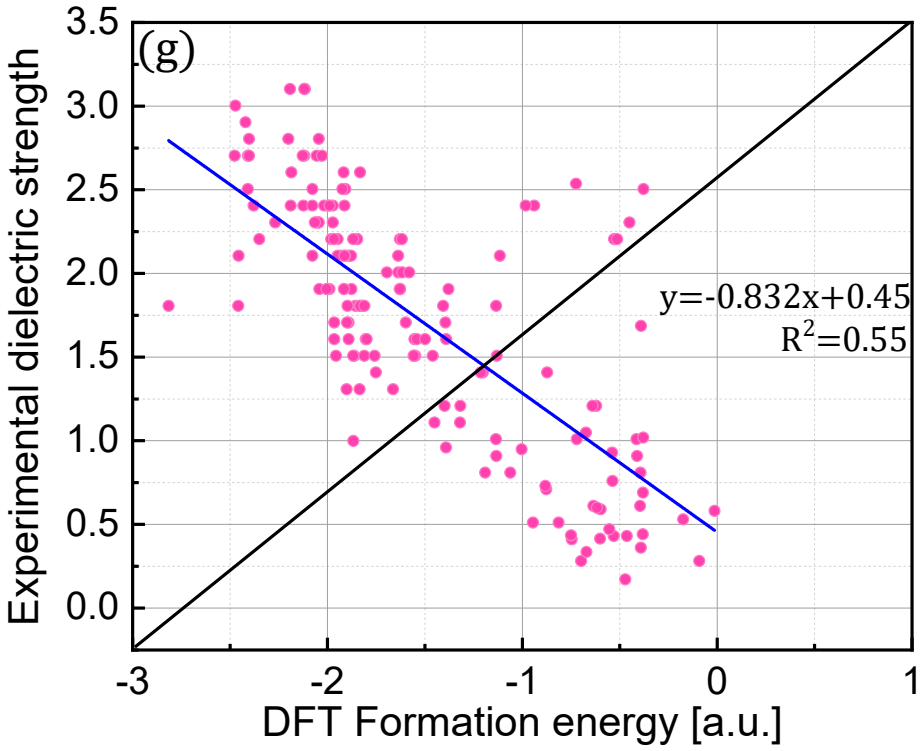

(b)
Experimental dielectric strength
DFT Calculated ε_i^a [eV]
y=-0.053x+2.325
R^2=0.005
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4
6
8
10
12
14
16

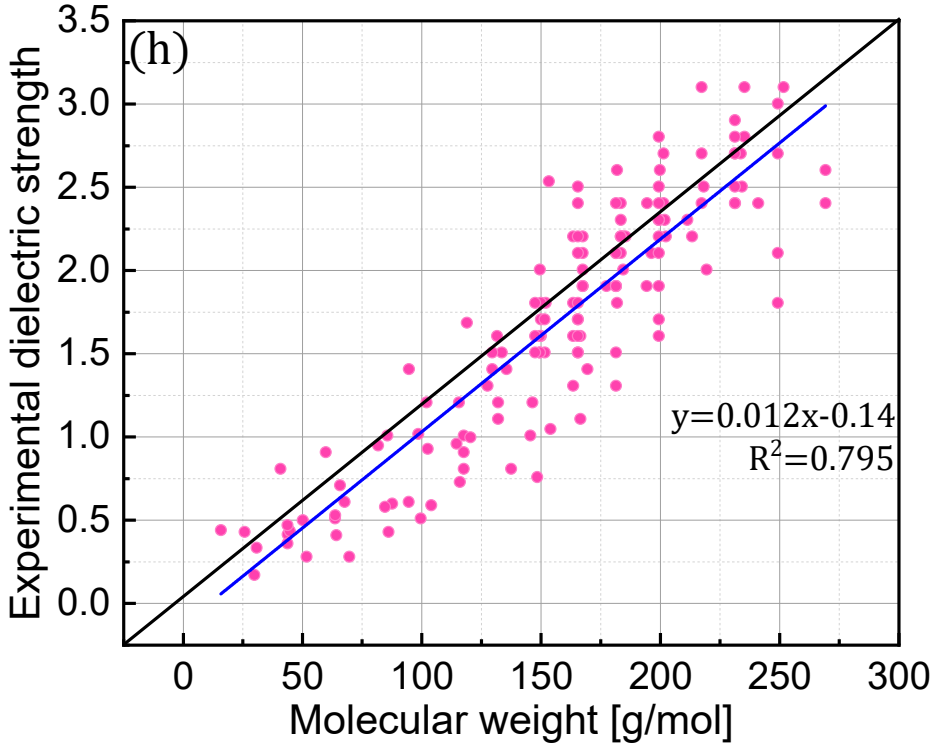

(c)
Experimental dielectric strength
The number of electrons (N_e)
y=0.025x-0.208
R^2=0.81
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140


(d)
Experimental dielectric strength
DFT HOMO [eV]
y=-0.176x-0.046
R^2=0.044
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
-14
-12
-10
-8
-6
-4


(e)
Experimental dielectric strength
DFT HOMO-LUMO Gap [eV]
y=-0.03x+2.014
R2=0.004
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4
6
8
10
12
14
16


(f)
Experimental dielectric strength
DFT Electronic spatial extent gap [a.u.]
y=0.028x+1.405
R2=0.041
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
5
10
15
20
25
30


(g)
Experimental dielectric strength
DFT Formation energy [a.u.]
y=-0.832x+0.45
R2=0.55
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-3
-2
-1
0
1


(h)
Experimental dielectric strength
Molecular weight [g/mol]
y=0.012x-0.14
R2=0.795
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
50
100
150
200
250
300

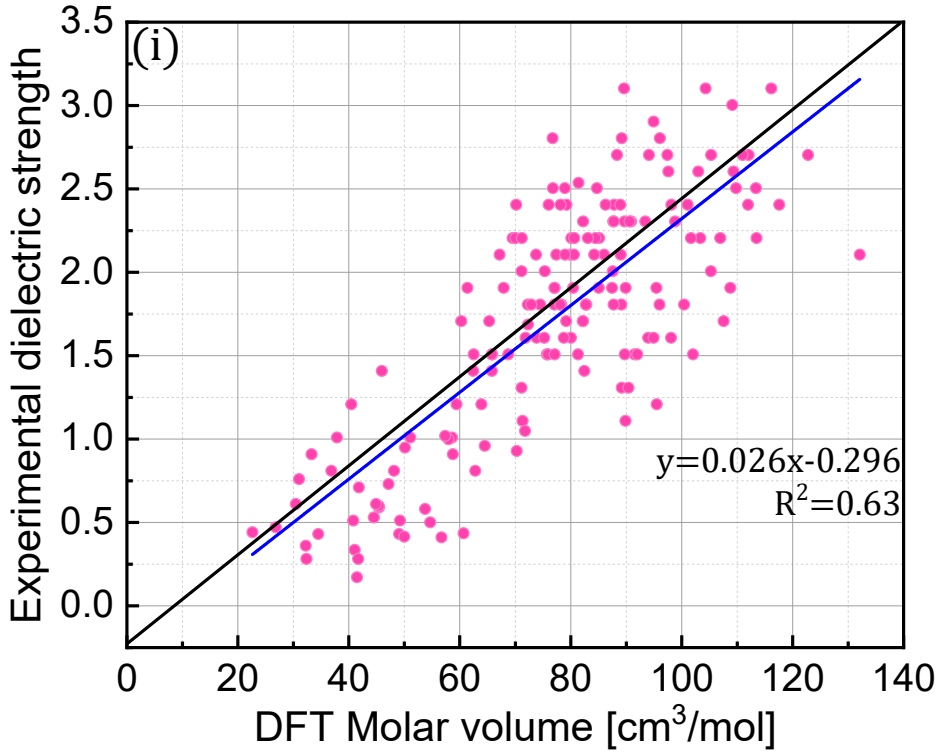


Figure S3. Correlations of experimental dielectric strength with (a) DFT-computed polarizability, (b) DFT-computed ionization energy, (c) the number of electrons, (d) DFT-computed HOMO, (e) DFT-computed HOMO-LUMO gap, (f) DFT-computed electronic spatial extent gap, (g) DFT-computed formation energy, (h) molecular weight, and (i) DFT-computed molar volume.

Table S1. Chemical formula and IUPAC name for each of 150 PFC compounds drawn in Figure S1.

No.	Formula	IUPAC name
1	C2F4	Tetrafluoroethylene
2	C2F6S	Bis(trifluoromethyl) sulfide
3	C2H2F2	1,2-Difluoroethene
4	C2H2F4O	1,2,2,2-Tetrafluoroethanol
5	C2H2F4O	Tetrafluoroethanol
6	C2H3F3O	1,1,2-Trifluoroethanol
7	C2H4F2	1,2-Difluoroethane
8	C2H4F2O	1,1-difluoroethanol
9	C2HBr2F3	2,2-dibromo-1,1,1-trifluoroethane
10	C2HBrF4O	2-Bromo-1,1,2,2-tetrafluoroethanol
11	C2HClF4O	2-Chloro-1,1,2,2-tetrafluoroethanol
12	C2HF5O	1,1,2,2,2-Pentafluoroethanol
13	C2HF5S	1,1,2,2,2-Pentafluoroethanethiol
14	C3F8S	(Trifluoromethyl)-(pentafluoroethyl) sulfide
15	C3H2F6O	(2S)-1,1,1,2,3,3-Hexafluoropropan-2-ol
16	C3H2F6O	1,1,1,3,3,3-Hexafluoro-2-propanol

17	C3H2F6O	(2R)-1,1,1,2,3,3-Hexafluoropropan-2-ol
18	C3H2F6O	1,1,1,2,3,3-Hexafluoro-2-propanol
19	C3H2F6O	Hexafluoro-1-Propanol
20	C3H2F6O	1,1,2,3,3,3-Hexafluoropropan-1-ol
21	C3H2F7N	1,1,1-Trifluoro-N-(fluoromethyl)-N-(trifluoromethyl)methanamine
22	C3H2F7N	Bis(difluoromethyl)(trifluoromethyl)amine
23	C3H3BrF4	2-Bromo-1,1,1,3-tetrafluoropropane
24	C3H3ClF4	3-Chloro-1,1,1,3-tetrafluoropropane
25	C3H3ClF4	2-Chloro-1,1,1,3-tetrafluoropropane
26	C3H3ClF4	2-chloro-1,1,3,3-tetrafluoropropane
27	C3H3F5	(2R)-1,1,1,2,3-Pentafluoropropane
28	C3H3F5	1,1,1,2,3-Pentafluoropropane
29	C3H3F5O	1,1,1,3,3-Pentafluoropropan-2-ol
30	C3H3F5O	2,2,3,3,3-Pentafluoro-1-propanol
31	C3H3F5O	1,2,3,3,3-Pentafluoropropan-1-ol
32	C3H3F5O	3-Pentafluoropropanol
33	C3H3F5O	Pentafluoro isopropanol
34	C3H3F5O	1,1-Difluoro-2-(trifluoromethoxy)ethane
35	C3H3F6N	N-(Difluoromethyl)-1,1,1-trifluoro-N-(fluoromethyl)methanamine
36	C3H3F6N	N,N-bis(difluoromethyl)-1,1-difluoromethanamine
37	C3H4ClF3	1-chloro-1,1,3-trifluoropropane
38	C3H4ClF3	1-chloro-1,3,3-trifluoropropane
39	C3H4F4	1,1,1,3-tetrafluoropropane
40	C3H4F4	1,1,3,3-tetrafluoropropane
41	C3H4F4O	1,1,3,3-Tetrafluoropropan-1-ol
42	C3HCl2F5O	1-(Dichloromethoxy)-1,1,2,2,2-pentafluoroethane
43	C3HClF6O	1-chloro-1,1,2,3,3,3-hexafluoropropan-2-ol
44	C3HF7O	1,1,2,2,3,3,3-heptafluoropropan-1-ol
45	C3HF8N	N-(difluoromethyl)-1,1,1-trifluoro-N-(trifluoromethyl)methanamine
46	C4F10S	Bis(perfluoroethyl)-sulphide
47	C4F10S	(Heptafluoropropyl)-(trifluoromethyl) sulfide
48	C4F4N2	2,3,5,6-Tetrafluoropyrazine
49	C4F6O	Hexafluoro-2,5-dihydrofuran
50	C4F8	Perfluoroisobutylene
51	C4F8	Octafluoro-2-butene
52	C4F8	Perfluoro-2-butene, (Z)-
53	C4F8	Octafluorobut-2-ene
54	C4F8S	Octafluorotetrahydrothiophene
55	C4H2ClF7O	2-[chloro(fluoro)methoxy]-1,1,1,3,3,3-hexafluoropropane
56	C4H2F6	1,1,1,4,4,4-Hexafluoro-2-Butene
57	C4H2F6	1,1,1,4,4,4-Hexafluorobut-2-ene
58	C4H2F6	3,3,3-Trifluoro-2-(trifluoromethyl)propene
59	C4H2F6	(2Z)-1,1,1,4,4,4-Hexafluorobut-2-ene
60	C4H2F6	1,1,1,2,4,4-Hexafluorobut-2-ene
61	C4H2F6	(E)-1,1,2,3,4,4-Hexafluorobut-2-ene
62	C4H2F8	1,1,1,2,3,3,3-Heptafluoro-2-(fluoromethyl)propane

63	C4H2F8	2-(Difluoromethyl)-1,1,1,2,3,3-hexafluoropropane
64	C4H2F8O	2-(Difluoromethyl)-1,1,1,3,3,3-hexafluoropropan-2-ol
65	C4H2F8O	1,1,1,2,3,3,4,4-Octafluorobutan-2-ol
66	C4H2F8O	1,1,1,3,3,4,4,4-Octafluoro-2-butanol
67	C4H2F8O	1,1,2,2,3,3,4,4-Octafluorobutan-1-ol
68	C4H3ClF6	2-Chloro-1,1,1,4,4,4-hexafluorobutane
69	C4H3F7	1,1,1,2,3,3,3-Heptafluoro-2-methylpropane
70	C4H3F7	1,1,1,3,3,3-Hexafluoro-2-(fluoromethyl)propane
71	C4H3F7	1,1,1,2,3,3-Hexafluoro-2-(fluoromethyl)propane
72	C4H3F7	2-(Difluoromethyl)-1,1,2,3,3-pentafluoropropane
73	C4H3F7	1,1,1,2,2,3,4-Heptafluorobutane
74	C4H3F7	2-Difluoromethyl-1,1,1,3,3-pentafluoropropane
75	C4H3F7O	2-(Trifluoromethyl)-2,3,3,3-tetrafluoro-1-propanol
76	C4H3F7O	Ethane, 1,1,1,2,2-pentafluoro-2-(2,2-difluoroethoxy)-
77	C4H3F7O	Sevoflurane
78	C4H3F7O	2-Difluoromethyl-1,1,1,3,3-pentafluoro-2-propanol
79	C4H3F7O	1,1,1,3,4,4,4-Heptafluorobutan-2-ol
80	C4H3F7O	1,1,2,2,4,4,4-Heptafluorobutan-1-ol
81	C4H3F7O	1,2,3,3,4,4,4-Heptafluorobutan-1-ol
82	C4H3F7O	1,1,2,2,3,3,4-Heptafluorobutan-1-ol
83	C4H3F7O	1,1,1,3-Tetrafluoro-3-(trifluoromethoxy)propane
84	C4H3F7O	1,1,1,2-Tetrafluoro-3-(trifluoromethoxy)propane
85	C4H4ClF5	1-Chloro-1,1,3,3,3-pentafluoro-2-methylpropane
86	C4H4ClF5	2-Chloro-1,1,1,2,4-pentafluorobutane
87	C4H4F4	(E)-1,2,3,4-Tetrafluorobut-2-ene
88	C4H4F6	1,1,1,3,3,3-Hexafluoro-2-methylpropane
89	C4H4F6	1,1,1,2,3,3-Hexafluoro-2-methylpropane
90	C4H4F6	1,1,1,4,4,4-Hexafluorobutane
91	C4H4F6	1,1,1,2,2,4-Hexafluorobutane
92	C4H4F6	1,1,1,3,3-Pentafluoro-2-(fluoromethyl)propane
93	C4H4F6	1,1,1,2,3,4-Hexafluorobutane
94	C4H4F6	1,1,2,3,3-Pentafluoro-2-(fluoromethyl)propane
95	C4H4F6	1,1,1,2,4,4-Hexafluorobutane
96	C4H4F6	1,1,1,2,4,4-hexafluorobutane
97	C4H4F6	1,1,1,3,4,4-hexafluorobutane
98	C4H4F6	1,1,2,2,3,4-hexafluorobutane
99	C4H4F6	1,1,2,3,4,4-hexafluorobutane
100	C4H4F6O	3,3,3-Trifluoro-2-(trifluoromethyl)propan-1-ol
101	C4H4F6O	1,1,1-Trifluoro-3-(trifluoromethoxy)propane
102	C4H4F6O	2-Difluoromethyl-1,1,3,3-tetrafluoro-2-propanol
103	C4H4F6O	1,1,1,2,2-Pentafluoro-2-(1-fluoroethoxy)ethane
104	C4H5F5	1,1,1,2,3-Pentafluoro-2-methylpropane
105	C4H5F5	1,1,1,4,4-Pentafluorobutane
106	C4H5F5	1,1,1,3,3-Pentafluoro-2-methylpropane
107	C4H5F5	1,1,1,3-Tetrafluoro-2-(fluoromethyl)propane
108	C4H5F5	1,1,2,3-Tetrafluoro-2-(fluoromethyl)propane
109	C4H5F5	1,1,3,3-Tetrafluoro-2-(fluoromethyl)propane
110	C4H6F4	1,1,1,3-Tetrafluorobutane
111	C4H6F4	1,1,1,3-Tetrafluoro-2-methylpropane
112	C4HClF8O	1-Chloro-1,1,3,3,3-pentafluoro-2-(trifluoromethyl)propan-2-ol
113	C4HF7	Tetrafluoro-2-(trifluoromethyl) propene
114	C4HF7	1,1,1,2,4,4,4-Heptafluoro-2-butene
115	C4HF7	(E)-1,1,1,2,4,4,4-Heptafluorobut-2-ene
116	C4HF7	1,1,1,2,4,4,4-Heptafluorobut-2-ene

117	C4HF7	1,3,3,3-Tetrafluoro-2-(trifluoromethyl)propene
118	C4HF9O	Perfluoro-tert-butanol
119	C4HF9O	Perfluorobutanol
120	C5F10	1,1,3,3,4,4,4-Heptafluoro-2-(trifluoromethyl)but-1-ene
121	C5F10	1,1,1,2,4,4,4-Heptafluoro-3-(trifluoromethyl)but-2-ene
122	C5F10	1,1,1,2,3,4,4,5,5,5-Decafluoropent-2-ene
123	C5F10	2-Pentene, 1,1,1,2,3,4,4,5,5,5-decafluoro-
124	C5F10	(Z)-1,1,1,2,3,4,4,5,5,5-Decafluoropent-2-ene
125	C5F8	Octafluorocyclopentene
126	C5H2F8	(2E)-1,1,1,4,4,5,5,5-Octafluoropent-2-ene
127	C5H2F8	1,1,1,4,4,5,5,5-Octafluoropent-2-ene
128	C5HF9	1,1,1,3,4,4,5,5,5-Nonafluoropent-2-ene
129	C5HF9	1,1,1,2,4,4,5,5,5-Nonafluoro-2-pentene
130	C5HF9	1,1,1,4,4,4-Hexafluoro-2-(trifluoromethyl)but-2-ene
131	C5HF9	(E)-1,1,1,3,4,4,5,5,5-Nonafluoropent-2-ene
132	C5HF9	(2E)-1,1,1,2,4,4,5,5,5-Nonafluoropent-2-ene
133	C5HF9	(E)-1,1,1,2,3,4,4,5,5-Nonafluoropent-2-ene
134	CH2F2O	Difluoromethanol
135	CHBrF2O	Difluorobromomethanol
136	CHClF2O	Chloro(difluoro)methanol
137	CHF3O	Trifluoromethanol
138	C2F3Cl	1-Chloro-1,2,2-trifluoroethene
139	C2F5Cl	1-Chloro-1,1,2,2,2-pentafluoroethane
140	C2F6	1,1,1,2,2,2-Hexafluoroethane
141	C4F7N	2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanenitrile
142	CF2Cl2	Difluorodichloromethane
143	CF3Br	Trifluorobromomethane
144	CF3Cl	Trifluorochloromethane
145	CF4	Tetrafluoromethane
146	CH2F2	Methylene difluoride
147	CHF2Cl	Difluorochloromethane
148	CHFCl2	dichloro(fluoro)methane
149	CHF3	Fluoroform
150	CF3CN	Trifluoroacetonitrile

Table S2. Chemical formula and IUPAC name for each of 18 non-PFC compounds drawn in Figure S2.

No.	Formula	IUPAC name
1	C2H2	Acetylen
2	C2H4O	1,2-Epoxyethane
3	C2H5Cl	Chloroethane
4	C2H7N	N-Methylmethanamine
5	CCl4	Tetrachloromethane
6	CH3Br	Bromomethane
7	CH3CHCl2	Ethylidene chloride
8	CH3Cl	Chloromethane
9	CH3CN	Cyanomethane
10	CH3NH2	Methanamine

11	CH4	methane
12	CHCl3	Trichloromethane
13	CO2	carbon dioxide
14	COS	Carbon oxide sulfide
15	N2O	Nitroous Oxide
16	C2H6	Ethane
17	CH2Cl2	Methylene dichloride
18	SO2	Sulfur Dioxide