Table S1 Experimental data of mass fraction (M_f), filler size (L), thicknesses (d_T), switching field (E_S), and nonlinear coefficient (α) of graphene-based composites with different polymer matrix extracted from relevant literature on nonlinear conductive composites.

	M_f (wt.%)	L (um)	d_T (mm)	E_S (kV/mm)	α
GN/PDMS	2.91	0.5	1	3.52	9.22
GN/PDMS	4.76	0.5	1	1.75	13.8
GN/SiR	50	–	1	3.98	3.13
GN/SiR	1	–	1	3.79	3.67
GN/SiR	3	–	1	2.65	4.2
GN/SiR	5	–	1	2.50	5.12
GN/SiR	4	25	1	0.41	2.04
GN/SiR	4.5	25	1	0.37	2.35
GN/SiR	5	25	1	0.25	2.48
GN/EP	3.4	12.5	10	0.12	1.25
GN/EP	3.09	12.5	10	0.11	1.32
GN/EP	2.92	12.5	10	0.10	1.20
GN/EP	2.69	12.5	10	0.87	1.44
GN/EP	2.35	12.5	10	0.80	2.14
GN/EP	2.06	12.5	10	0.67	3.23

Table S2 The DFT computed layer distance (d_L), binding energy (BE), charge transfer (e), and polymer band gap (P_{gap}) of polymer adsorbed on graphene layer. Please note that the data from Reference 8 is not full presented in Table S2 due to its large amount.

	d_L (Å)	BE (eV)	q (e)	P_{gap} (eV)
GN/PANI	2.910	-0.720	–	3.52
GN/PPy	3.500	-0.250	–	3.50
GN/TCNE	3.401	-0.233	-0.274	2.01
GN/TCNQ	3.497	-0.255	-0.263	0.81
GN/F4TCNQ	3.508	-0.635	-0.506	0.62
GN/TDAE	3.082	-0.417	0.454	1.21
GN/ANTR	3.748	-0.151	0.002	0.20
GN/$GeF_2SnCl_2SiCl_2CH_2$	–	-1.180	0.095	1.42
GN/$GeCl_2SnCl_2SiCl_2CH_2$	–	-1.366	0.027	1.18
GN/$GeF_2SnF_2SiF_2CH_2$	–	-1.373	0.009	1.45
GN/$GeCl_2SnF_2SiCl_2CH_2$	–	-1.179	0.017	1.66

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References

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Table S3 The 30 raw input features before the feature engineering step.

Label	Features	Label	Features
MW	MolecularWeight	B_s	BondStereoCount
HB_d	HBondDonorCount	V_{3D}	Volume3D
HB_a	HBondAcceptorCount	Q_X	XStericQuadrupole3D
XLogP	XLogP	Q_Y	YStericQuadrupole3D
E_m	ExactMass	Q_Z	ZStericQuadrupole3D
M_m	MonoisotopicMass	F_C	FeatureCount3D
TPSA	TPSA	F_A	FeatureAcceptorCount3D
C	Complexity	F_d	FeatureDonorCount3D
Q	Charge	F_a	FeatureAnionCount3D
H_a	HeavyAtomCount	F_{cc}	FeatureCationCount3D
R_b	RotatableBondCount	F_r	FeatureRingCount3D
I_a	IsotopeAtomCount	F_h	FeatureHydrophobeCount3D
A_s	AtomStereoCount	C_m	ConformerModelRMSD3D
D_a	DefinedAtomStereoCount	E_r	EffectiveRotorCount3D
U_a	UndefinedAtomStereoCount	C_c	ConformerCount3D

Table S4 186 polymer monomers were acquired from the PubChem database for machine learning training of Py/GN composites.

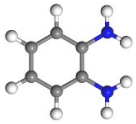
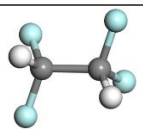
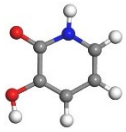
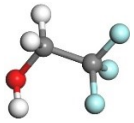
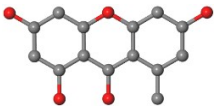
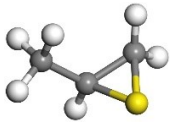
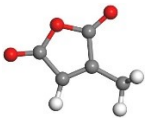
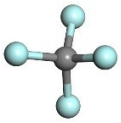
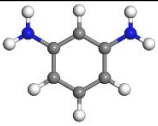
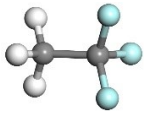
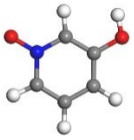
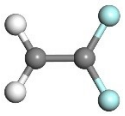
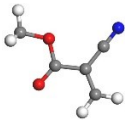
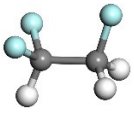
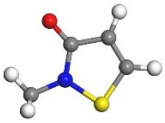
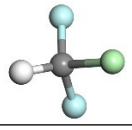
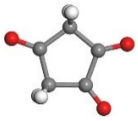
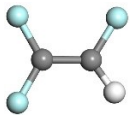
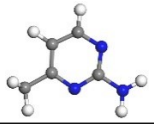
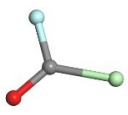
No.	CID	Molecular Formula	E_b (V/ Å)	No.	CID	Molecular Formula	E_b (V/ Å)
1	126	C7H6O2	1.0	94	1207241	C13H13N	0.7
2	227	C7H7NO2	1.0	95	1207248	C12H11NO	0.7
3	241	C6H6	1.0	96	1413561	C8H6N4	0.5
4	261	C4H8O	1.3	97	2723704	C2H6N2S	1.3
5	460	C7H8O2	1.0	98	2759342	C7H7NOS	0.6

6	702	C2H6O	1.0	99	3034616	CH4N2OS	0.8
7	887	CH4O	1.2	100	3034652	C8H9NS	0.6
8	904	C8H9NO	1.0	101	4192173	CH3NO3	1.4
9	996	C6H6O	0.6	102	4686860	C4H6O2	1.4
10	1031	C3H8O	1.7	103	5246501	C2H7NO	1.3
11	1032	C3H6O2	1.4	104	5252227	C2H4O2S	1.3
12	3657	CH4N2O2	1.4	105	5256157	C2H8N2	1.3
13	5147	C7H7NO2	1.0	106	7183284	C12H10OS	0.6
14	5798	C7H6N2	0.5	107	10868587	C18H14O	0.9
15	6154	C24H36FNO	0.9	108	10986946	C13H13N	1.0
16	6325	C2H4	1.7	109	11159903	C14H12O	0.6
17	6337	C2H5Cl	1.3	110	11322869	C19H14O	0.6
18	6373	CHF3	1.8	111	11769329	C11H10OS	0.9
19	6557	C5H8	0.7	112	11788313	C7H9NO	1.1
20	6579	C3H5NO	1.0	113	12106420	C8H8OS	0.6
21	6581	C3H4O2	1.5	114	12412244	C3H5NO2	1.3
22	6658	C5H8O2	1.1	115	12454639	C2H3NO2S	0.7
23	6809	C8H5NO2	0.5	116	12463483	C4H8S	0.8
24	6994	C8H10O	1.0	117	12595497	C18H15N	0.6
25	6997	C8H10O	1.0	118	12750541	C11H9NOS	0.5
26	7148	C9H10O	1.0	119	12859659	C3H5NOS	0.7
27	7222	C7H5NS	0.4	120	12993673	C6H6O2S	1.0
28	5801	C6H7NO	0.2	121	13288501	C3H7NS	1.3
29	7407	C9H10	0.4	122	13316132	C3H7NO	1.3
30	7501	C8H8	1.0	123	13433468	C14H12S	0.6
31	7668	C9H12	1.1	124	13586586	C6H9NS	1.1
32	7669	C8H11N	1.1	125	13738548	C7H6O3	0.6
33	7670	C8H11N	1.1	126	13794763	C7H6O2S	1.1
34	7678	C9H10O	1.1	127	14591620	C6H6O2S	1.1
35	7809	C8H10	0.7	128	14792808	C3H4O2S	0.7
36	7843	C4H10	1.3	129	14900621	C19H16	0.9
37	7852	C3H9N	1.3	130	15164605	C2H5NOS	1.2
38	7855	C3H3N	1.4	131	15322164	C13H12O	1.0
39	8024	C4H6O	0.4	132	15387271	C2H3NO2S	0.7
40	8027	C4H5N	0.5	133	15593934	C13H10O2	0.6
41	8252	C3H6	1.2	134	17883889	CH3NO2S	1.2
42	8255	C4H8	1.0	135	17976708	C7H7NOS	0.6
43	8299	C3H6O2	1.4	136	18364271	C3H4O2S	0.7
44	8373	C8H8O2	1.0	137	18440791	C4H6OS	0.7
45	8375	C8H8O2	1.0	138	18763820	C2H3NO3	1.3
46	8406	C8H6O3	1.0	139	18934690	C8H7NOS	0.6
47	8821	C5H8O2	1.4	140	19068320	C3H6OS	0.7
48	9253	C5H10	1.3	141	19072905	C5H6N2OS	0.6

49	9256	C3H3NS	1.1	142	19091706	C9H10S	0.6
50	9620	C2H5F	1.5	143	19788377	C8H9NS	0.6
51	6388	C2H3ClF2	1.8	144	19857337	CH5NO2	1.4
52	11908	C7H9NO	1.0	145	19893156	C11H10OS	1.0
53	11954	C8H9NO	1.0	146	20200291	C13H11NS	0.6
54	12332	C6H13NO	0.2	147	20469232	C4H6OS	0.7
55	12549	C24H18	0.6	148	20548556	C4H6S2	0.6
56	13140	C3H3ClO	1.5	149	20631564	C6H8OS	0.6
57	15742	C14H14	1.0	150	21063999	C8H9NS	1.0
58	21716	C6H6O2S	0.6	151	21226150	C6H7NO2	1.0
59	31229	C8H8O2	1.1	152	21916651	C13H10OS	0.6
60	31369	C4H5Cl	0.8	153	22181936	C17H12S2	0.6
61	31386	C12H10O2S	0.6	154	22311450	C6H8N2O	1.0
62	62540	C2H6O2	1.4	155	22463668	C3H5NOS	0.7
63	67230	C14H12O	1.0	156	23173285	C2H3NO2S	0.7
64	68297	C12H12N2	0.6	157	24723385	C12H10OS	0.9
65	69138	C7H9NO	1.0	158	53642269	C13H11NS	0.6
66	69322	C7H7NO2	1.1	159	54013827	C2H4N2OS	0.7
67	69357	C2H7NO	1.3	160	54228456	C8H7NOS	0.6
68	69738	C14H14	1.0	161	54480832	C12H12S	0.6
69	70922	C2H4N2O2	1.3	162	55284962	C5H8N2S	1.0
70	74690	C3H6OS	1.3	163	56622474	C9H8OS	0.6
71	75269	C3H4O3	1.3	164	56991064	C11H9NOS	0.6
72	75491	C12H10O2	1.0	165	57100077	C2H2O3S	1.2
73	75899	C12H11NO	0.7	166	66352987	C10H10N2S	0.6
74	76080	C13H11NO	1.0	167	69259074	C5H5NO2S	0.8
75	78498	C7H10N2	1.0	168	69333801	C5H6O2S	1.1
76	83254	C13H11NO	0.6	169	80231965	C10H8OS2	0.6
77	88060	C13H10O2	0.7	170	83390159	C6H7NS2	0.6
78	97310	C6H7NOS	1.1	171	83619751	C10H9NOS	1.0
79	119391	C2H2N2S	1.5	172	85575091	C12H12S	1.0
80	151196	C8H7NO2	0.6	173	85599492	C8H6O2S	0.6
81	152671	C9H8O2	0.7	174	85931947	C2H4N2S2	0.7
82	161195	C14H10O2	0.6	175	88131928	C3H4O2S	1.2
83	181496	C2H5NOS	1.3	176	91316097	C3H7NS	0.8
84	267569	C8H9NO	0.6	177	123659634	C11H11NS	0.6
85	458663	C5H5NO2S	0.6	178	135075782	C12H10OS	0.6
86	519073	C7H10S	1.2	179	135973227	C8H8OS	0.6
87	529944	C7H8OS	0.7	180	136168676	C3H2O3S	0.6
88	529949	C7H8OS	1.2	181	136378294	C13H10OS	0.6
89	542733	C2H5NO2	1.3	182	142065278	C7H6O2S	0.6
90	676454	C7H8N2S	0.6	183	143125387	C8H8OS	1.0
91	693140	C6H9NS	1.2	184	143219602	C11H9NOS	0.6

92	818884	C6H4O3S	0.7	185	143697997	C6H8OS	1.0
93	819553	C6H7NOS	1.1	186	154074681	C3H5NOS	0.6

Table S5 Among the 33375 predicted polymer molecules, (CID-1) 10 polymer molecules with lower E_b values, and (CID-2) 10 polymer molecules with higher E_b values were screened.

CID-1	Molecular structure	Molecular Formula	CID-2	Molecular structure	Molecular Formula
7243		C6H8N2	9667		C2H2F4
28115		C5H5NO2	6409		C2H3F3O
12273		C5H5NO2	14072		C3H6S
12012		C5H4O3	6393		CF4
7935		C6H8N2	9868		C2H3F3
23069		C5H5NO2	6369		C2H2F2
8711		C5H5NO2	9890		C2H3F3
39800		C4H5NOS	6372		CHClF2
27507		C5H4O3	9665		C2HF3
7939		C5H7N3	9622		CClFO

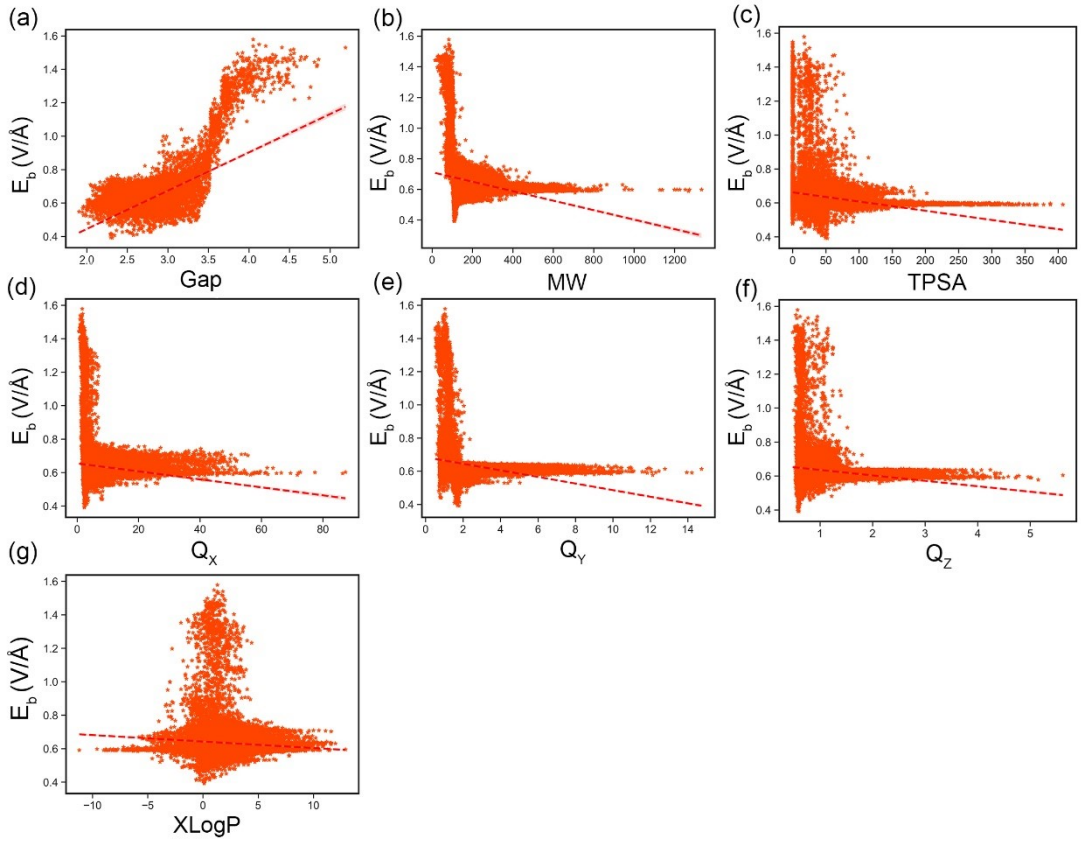


Fig S1 Scatter plots on E_b for 7 input features acquired from the PubChem database.