Supplementary Information

Harnessing Machine Learning to Probe Dielectrics in Next Generation Telecommunication and Automotive Radar Applications

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Table S1: The synthesis parameters for $Ba_3(VO_4)_2$-doped Mg_2SiO_4 used as the original input data for the machine learning model, were obtained through the solid-state reaction method.

					Input variables						Output variable
Mg/Si ratio	**Impurity**	**Compound**	**$Ba_3(VO_4)_2$ doping amount**	**Sintering time (hr)**	**Sintering temperature (℃)**	**Proportion**	**Sintered Density**	**Test frequency (GHz)**	**Dielectric Constant**	**Dielectric loss**	**Experimental Q×f value**
2	N	Y	50	4	1175	50	97.6	11.3	9.48	0.0004	46600
2	N	Y	45	4	1175	55	97	11.3	9.03	0.0004	52500
2	N	Y	40	4	1200	60	97.3	11.3	8.81	0.0004	55900
2	N	Y	35	4	1200	65	97	11.3	8.44	0.0004	52200

Table S2: The synthesis parameters for LiF-doped Mg_2SiO_4 used as the original input data for the machine learning model, were obtained through the solid-state reaction method.

					Input variables						Output variable
Mg/Si ratio	**Impurity**	**Compound**	**LiF doping amount**	**Sintering time (hr)**	**Sintering temperature (℃)**	**Proportion**	**Sintered Density**	**Test frequency (GHz)**	**Dielectric Constant**	**Dielectric loss**	**Experimental Q×f value**
2	N	Y	0.5	4	1200	99.5	97.1	12.8	6.98	0.002	171000
2	N	Y	1	4	950	99	97	12.8	7.02	0.002	162300
2	N	Y	2	4	800	98	97	12.8	6.81	0.002	167000
2	N	Y	3	4	800	97	97	12.8	6.95	0.002	160300

Table S3: The synthesis parameters for LMZBS-doped Mg_2SiO_4 used as the original input data for the machine learning model, were obtained through the solid-state reaction method.

Impurity	Compound	LMZBS addition amount	Sintering time (hr)	Input variables							Output variable
				Mg/Si ratio	Sintering temperature (°C)	Proportion	Sintered Density	Test frequency (GHz)	Dielectric Constant	Dielectric loss	Experimental Q×f value
Y	N	0	3	2	1400	100	97.2	10.76	7.24	0.0022	54820
Y	N	0	3	2.025	1400	100	97.2	10.85	7.43	0.0018	73620
Y	N	0	3	2.05	1400	100	97.2	10.57	7.5	0.0016	114730
Y	N	0	3	2.2	1400	100	97.2	10.45	7.59	0.0013	107370
N	N	0	3	2	1075	100	92.6	11.35	7.2	0.0022	193800
Y	N	0	2	2	1400	100	96.7	16	6.8	0.000066	240000
N	N	0	2	2	1550	100	95	13	7.1	0.002	168400
Y	Y	0.5	2	2	1525	99.5	97	13	7.3	0.001	198503.4
Y	Y	1	2	2	1375	99	96	13	7.2	0.001	190574.2
Y	Y	3	2	2	1250	97	96	13	7.15	0.001	203276.5
Y	Y	5	2	2	1250	95	95	13	6.9	0.002	181046.3
Y	Y	10	2	2	1000	90	93	13	6.76	0.002	217718.7
Y	Y	15	2	2	950	85	91	13	6.75	0.003	30600

Table S4: The synthesis parameters for MgO-doped Zn_2SiO_4 used as the original input data for the machine learning model, were obtained through the solid-state reaction method.

MgO addition amount	Input variables				Compound	Impurity	Sintering time (hr)	Output variable
	Zn/Si ratio	Proportion	Sintering temperature (°C)	Dielectric Constant				Experimental Q×f value
0	2	100	1250	6.4	N	N	3	108000
10	2	90	1250	6.5	Y	N	3	21500
20	2	80	1250	6.385	Y	N	3	38500
30	2	70	1250	6.245	Y	N	3	73021
40	2	60	1250	6.097	Y	N	3	129991
50	2	50	1250	6.52	Y	N	3	98500
0	1.8	100	1300	6.6	N	Y	3	147000

Table S5: Fabrication parameters for antenna design through number of sides of polygon and thickness as the original input data for the machine learning model.

Input variables		Bandwidth (THz)	Lowest point (THz)	Bandwidth center point (THz)	Number of bands	Max Gain (dBi)	Output variable
Polygon sides	Thickness (m)						Efficiency (%)
3	0.0002	0.564	0.6	0.718	2	10.2	81.2
3	0.002	0.563	0.598	0.718	3	10.7	84.3
4	0.0002	0.6	0.663	0.7	4	11.3	94.4
4	0.002	0.47	0.466	0.765	4	11.3	82
5	0.0002	0.63	0.605	0.685	2	10.8	82
5	0.002	0.456	0.6	0.772	5	10.9	99.5
6	0.0002	0.461	0.8	0.769	2	12	79
6	0.002	0.451	0.595	0.774	3	10.9	79.4
7	0.0002	0.475	0.632	0.762	5	11.5	75
7	0.002	0.581	0.627	0.7	3	11.8	79.6
8	0.0002	0.434	0.635	0.783	7	13.3	112
8	0.002	0.579	0.9	0.71	1	12.9	81.8

Table S6: The synthesis parameters of polymers for antenna design used as the original input data for the machine learning model.

Polymer	Input variables				Glass transition temperature (℃)	χ (electronegativity)	Coefficient of expansion (ppm)	Test frequency	Output variables	
	Molecular Weight	Nc (Number of C-side chain)	Nb (Number of Benzene rings)	Moisture					Dielectric Constant	Dielectric loss (Q×f)
PMDA-6FDAM	223400	1	1	0.95%	282	43.6	**56.3**	1MHz	2.95	0.0035
6FDA-6FDAM	135200	3	1	0.42%	261	67.6	**82.5**	1MHz	2.71	0.0028
BTDA-6FDAM	190500	1	1	0.84%	238	47	**37.6**	1MHz	2.91	0.0031
ODPA-6FDAM	167500	1	1	0.52%	242	47	**37.6**	1MHz	2.89	0.0029
9FDA-4,4'-ODA	580000	3	1	0.35%	283.6	59	**26.8**	1MHz	2.89	0.0014
9FDA-APB	230000	3	1	0.18%	259.5	62.4	**44.2**	1MHz	2.97	0.0022
9FDA-3,4'-ODA	210000	3	1	0.40%	257.7	59	**26.8**	1MHz	2.88	0.0013
9FDA-9FAPB	280000	6	1	0.10%	245.8	86.4	**44.4**	1MHz	2.71	0.0028
BGTF-HMDA	**35561**	2	0	0.23%	175	28.56	**68.9**	1MHz	3.3	0.0028
BGTF-DDM	**20326**	2	1	0.13%	170	26.4	**68.2**	1MHz	3.2	0.0021
DGEBA-HMDA	**24006**	2	0	0.32%	164	21.76	**68.9**	1MHz	3.5	0.0073
DGEBA-DDM	**21817**	2	1	0.14%	187	19.6	**68.5**	1MHz	3.6	0.0069
ADEP	**160295**	16.8	0	1.68%	372	141.2	24	200MHz	3.07	**0.2212**
EP904	**255994**	9.6	0	1.99%	428	48.87	782	200MHz	3.63	**0.0096**
Silixane-ADEP	**250706**	9.6	0	2.08%	428	71.4	522	200MHz	4.54	**0.0096**
DGEBA/B10	**21691**	7.2	0	1.08%	223	36.6	**68.9**	10KHz	2.943	0.02
BP/B10	**172176**	2	0	1.23%	253	36.6	**68.5**	10KHz	2.638	0.001
FBE-FBP	**213540**	3	0	0.27%	424	34.2	**68.7**	1MHz	3.8	0.0036
FBE-BP	**200341**	3	0	0.33%	429	22.2	**68.9**	1MHz	4.1	0.0038
BE-FBP	**188094**	3	0	0.29%	438	22.2	**68.9**	1MHz	4.1	0.0045
BE-BP	**198362**	3	0	0.37%	431	10.2	**68.9**	1MHz	4.2	0.004

6FCDA/TFMB	215000	4.8	0	1.20%	420	77.8	6	1MHz	2.4	**0.0096**
6FCDA/TFMOB	217000	4.8	0	0.80%	375	84.6	10	1MHz	2.8	**0.2171**
6FCDA/TFEOB	205000	4.8	0	0.70%	363	92.6	10	1MHz	3	**0.0097**
6FCDA/DFPOB	106000	4.8	0	0.10%	350	147.4	109	1MHz	2.5	**0.0096**
3FCDA/TFMB	396000	3	0	1.90%	426	65.8	20	1MHz	2.7	**0.0096**
3FCDA/TFMOB	354000	3	0		400	72.6	36	1MHz	2.6	**0.0096**
3FCDA/TFEOB	203000	3	0	0.80%	378	80.6	40	1MHz	3.1	**0.0097**
PETI-PMDA (CH3)3	**108248**	0	0	0.45%	245	26.4	**68.9**	1MHz	3.17	0.24
PETI-PMDA (CH3)4	**85783**	0	0	0.48%	232	26.4	**68.9**	1MHz	3.06	0.19
PETI-PMDA (CH3)5	**76612**	0	0	0.56%	224	26.4	**68.9**	1MHz	2.82	0.31
PETI-PMDA (CH3)6	**62140**	0	0	0.40%	202	26.4	**68.9**	1MHz	2.77	0.26
Fn1-FDA	125000	2	2	0.80%	302	50.4	**64.3**	1MHz	2.49	0.0123
Fn2-FDA	181000	6	2	0.67%	311	50.4	**62.9**	1MHz	2.44	0.0064
Fn1-ODPA	107000	0	2	1.05%	296	29.8	**59.6**	1MHz	2.72	0.0099
Fn2-ODPA	180000	4	2	0.72%	322	29.8	**63.7**	1MHz	2.65	0.0118
Fn2-Si-ODPA	263000	4	6	0.45%	292	29.8	**62.7**	1MHz	2.75	0.0061
Fn2-Si-FDA	256000	6	6	0.19%	308	50.4	**62.7**	1MHz	2.63	0.0091
Fn2-Si-BPADA	180000	6	6	0.15%	245	33.2	**62.7**	1MHz	2.67	0.0024
LCPEI-10	33600	4.8	1	0.39%	218	9.185	58.1	10GHz	3.07	0.006
LCPEI-12.5	38000	4.8	1	0.55%	220	9.675	68.4	10GHz	2.91	0.008
LCPEI-3F	**39227**	4.8	1	0.44%	220	10.385	75.2	10GHz	3	0.0082
LCPEI-4F	**18203**	0	1	0.55%	191	10.785	78	10GHz	3.01	0.0063
LCPEI-6F	**47516**	7.2	1	0.33%	212	11.585	83.1	10GHz	2.93	0.0076
PEI-6F25AF	46200	7.2	1	0.42%	238	16.36	88.9	10GHz	2.6	0.0012
PEI-6Fd25AF	32700	4.8	0	0.46%	221	16.36	79.3	10GHz	2.79	0.0077

TABPFL-4,4'-ODA	**116760**	0	2	0.71%	299	43.4	62.5	1MHz	3.01	0.0144
TABPFL--p-PDA	**143475**	0	2	1.77%	324	40	58.3	1MHz	3.05	0.014
TABPFL-m-TOL	**152826**	2	2	0.80%	312	40	57.7	1MHz	3.07	0.0174
TABPFL-TFMB	**96677**	2	2	0.68%	309	64	61.6	1MHz	2.87	0.0161
TABPFL-MBCHA	**104350**	0	2	0.60%	290	40	62.4	1MHz	2.9	0.0105
TABCFL-4,4'-ODA	**113199**	2	2	0.83%	285	43.4	63.6	1MHz	3.09	0.0084
TABCFL-p-PDA	**152826**	2	2	1.15%	312	40	64.5	1MHz	3.07	0.0081
TABCFL-m-TOL	**122600**	4.8	2	0.99%	309	64	66.6	1MHz	2.97	0.0065
TABCFL-TMFB	**150139**	4.8	2	0.46%	293	40	64.3	1MHz	2.87	0.0111
TABCFL-MBCHA	**85847**	2	2	0.85%	277	40	67.2	1MHz	2.88	0.0113
CY-1	**204056**	7.2	2	1.91%	323	26.4	**64.2**	10GHz	2.84	0.0092
CY-1/6FDABPA	**266270**	14.4	2	1.89%	293	86.4	**61.8**	10GHz	2.81	0.0082
CY-1/Si-B	**259779**	14.4	6	0.73%	297	45.2	**62.7**	10GHz	2.95	0.0136
CY-1/Si/H	**237709**	12	6	1.71%	299	24.8	**62.7**	10GHz	2.81	0.0089

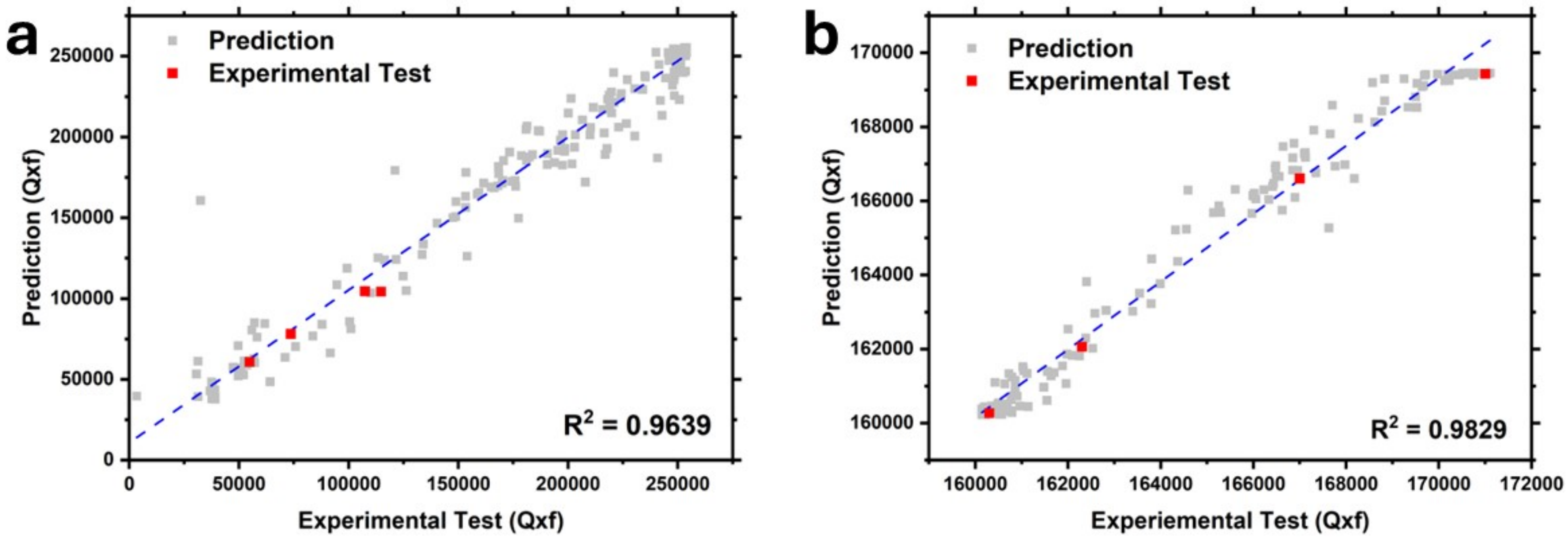

Figure S1: Experimental validation of the quality factors (Q×f) of Mg_2SiO_4 doped with $Ba_3(VO_2)_4$ **(a)** and LiF **(b)** compared to the generated prediction output.