Supplementary Materials

Interpretable model of dielectric constant for rational design of microwave dielectric materials: a machine learning study

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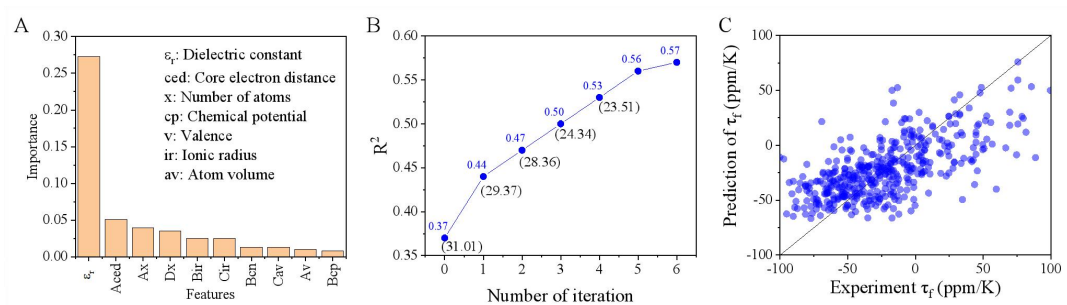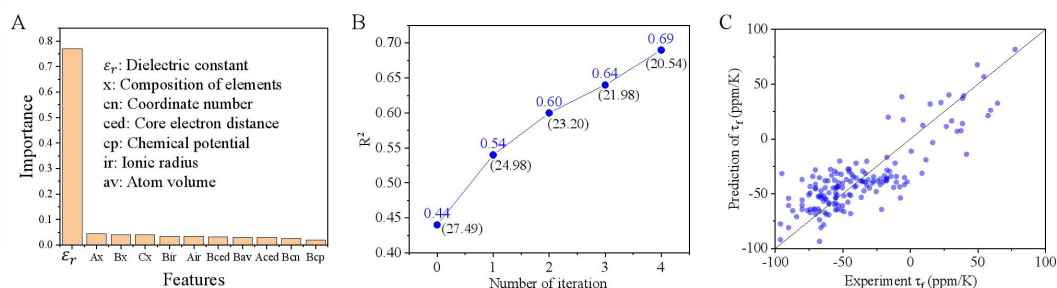
Supplementary Figure 1. Machine learning results of τ_f for quaternary materials. (A) RF ranking of importance of material features for τ_f in the quaternary materials. (B) Variation of R^2 and RMSE (in the black bracket) in the prediction model of τ_f as a function of iteration steps. (C) Scatter plot of predicted τ_f versus experimental values for the quaternary materials after six iterations.
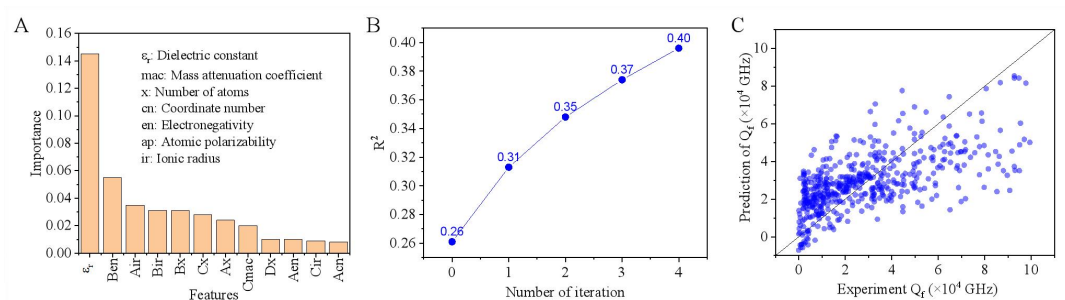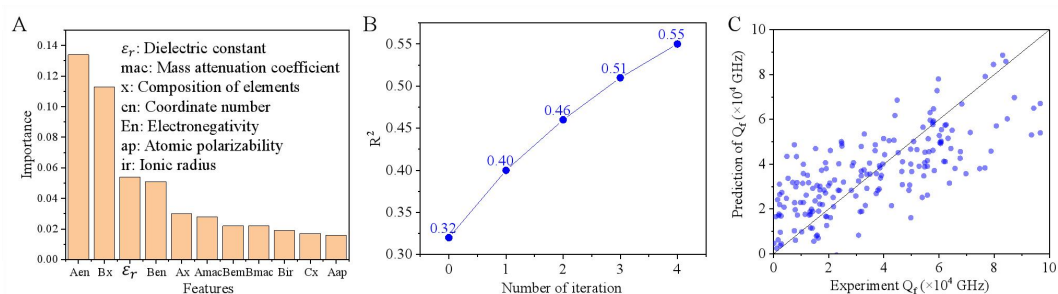
Supplementary Figure 2. Machine learning results of Q_f for quaternary materials. (A) RF ranking of importance of material features for Q_f in the quaternary materials. (B) Variation of R^2 in the prediction model of Q_f as a function of iteration steps. (C) Scatter plot of predicted Q_f versus experimental values for the quaternary materials after four iterations.
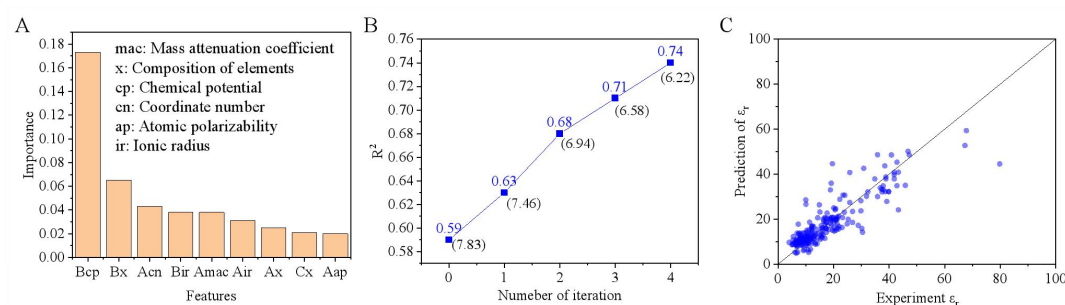
Supplementary Figure 3. Machine learning results of ε_r for ternary materials. (A) RF ranking of importance of material features for ε_r in the ternary materials. (B) Variation of R^2 and RMSE (in the black bracket) in the prediction model of ε_r as a function of iteration steps. (C) Scatter plot of predicted ε_r versus experimental values for the ternary materials after four iterations.

Supplementary Figure 4. Machine learning results of τ_f for ternary materials. (A) RF ranking of importance of material features for τ_f in the ternary materials. (B) Variation of R^2 and RMSE (in the black bracket) in the prediction model of τ_f as a function of iteration steps. (C) Scatter plot of predicted τ_f versus experimental values for the ternary materials after six iterations.

Supplementary Figure 5. Machine learning results of Q_f for ternary materials. (A) RF ranking of importance of material features for Q_f in the ternary materials. (B) Variation of R^2 in the prediction model of Q_f as a function of iteration steps. (C) Scatter plot of predicted Q_f versus experimental values for the ternary materials after four iterations.

The following are the predicted models (equations) in terms of the features of quaternary and ternary materials:

1, Prediction model of ε_r for quaternary materials:

$$\varepsilon_r = 0.164\,ln\,(C_{mac}) \cdot \left\{0.854 \cdot \frac{(C_{ap}+D_{ap})\cdot cos\,(A_x)}{C_{ap}} \cdot \left[0.31\frac{C_{cp}\cdot B_{cn}\cdot C_{mac}\cdot\sqrt{A_{ap}}}{e^{C_{cp}}} + 9 \times 10^{-2}D_x^4 \cdot \right.\right.$$
$$A_{cp} \cdot C_{ap} \cdot (A_{mac}+B_{mac}) + 3\Big] - 1.3 \times 10^{-4}\,cos\,(A_{ap}) \cdot cos\,(A_x) \cdot e^{B_{cn}} -$$
$$0.05\,cos\,(A_x) + 9\frac{A_{ap}\times B_{ir}\times C_{ir}}{B_{cn}\times C_{mac}\times D_x^3} - 1.26\Big\} + 3.1 \times 10^{-3}A_x \cdot (A_{mac}-C_{mac}) \cdot (4.6 \times$$
$$10^{-4}\frac{B_{cn}\cdot C_{mac}\cdot\sqrt{A_{ap}}\cdot A_{cp}\cdot C_{ap}\cdot(A_{mac}+B_{mac})}{D_{mac}^2} + 11\Big) + 1.4 \tag{1}$$

2, Prediction model of τ_f for quaternary materials:

$$\tau_f = 11.17\frac{(B_v+C_v)\cdot D_x\cdot A_v\cdot\varepsilon_r\cdot C_{ced}}{(A_{cp}+C_{cp})\cdot C_{av}} + 44.92\frac{(B_v+C_v)\cdot A_v\cdot D_x^2\cdot sin\,(A_{cn}\cdot A_{ir})}{A_{cp}+C_{cp}} + 1.69 \times$$
$$10^2\frac{D_x\cdot[B_v+A_v\cdot sin\,(B_{ir})]}{A_v\cdot(A_{cp}+C_{cp})} - \frac{364.72\cdot D_x}{(A_{cp}+C_{cp})} - 1.5 \times 10^{-2}\frac{(B_{av}-C_{av})\cdot(A_v+B_v)\cdot C_{ir}\cdot\varepsilon_r}{A_v} - 1.63(B_{av} -$$
$$C_{av}) \cdot C_{ir} - 4.44 \tag{2}$$

3, Prediction model of Q_f for quaternary materials:

$$Q_f = 1.2\frac{B_{ap}}{B_{ap}+D_{ap}} \cdot \left\{3.7\,ln\,(B_{aw}) \cdot \left\{0.3\frac{C_{cn}}{D_x\cdot C_{en}} \cdot \left[5.8 \times 10^5\left(\frac{C_{cn}\cdot(B_x+C_x)}{B_{ap}^2\cdot C_{en}\cdot B_{cn}\cdot\varepsilon_r}\right)^{\frac{1}{3}} + 27.9C_{cn}^6 \cdot\right.\right.\right.$$

$$B_{ap} \cdot \frac{A_x^6\cdot C_{mac}}{B_{ym}} - 4.7 \times 10^3\Big] + 3.5 \times 10^3\frac{B_{en}\cdot|A_{en}-C_{en}|}{C_{ap}} + 135.1\Big\} + 1.5 \times 10^4 B_x \cdot A_{ir} \cdot$$

$$B_{aw} \cdot \left(\frac{C_{cn}}{B_{ap}\cdot C_{en}\cdot\varepsilon_r}\right)^{\frac{1}{2}} \cdot \left(\frac{1}{C_{me}}\right)^{\frac{1}{3}} + 92.2B_x \cdot A_{ir} \cdot B_{aw} - 4.2 \times 10^3\Big\} + 2.4 \times 10^6\frac{B_x\cdot A_{cn}}{A_{ap}^6} -$$

$$1.5 \times 10^3 \tag{3}$$

4, Prediction model of ε_r for ternary materials：

$$\varepsilon_r = 0.76\frac{A_{ir}}{sin\,(A_{ir})}\Big\{0.87\frac{B_{mac}}{(B_{mac}+C_{mac})}\Big\{0.973\{(0.3\sqrt{A_{cn}} - 4.7 \times 10^{-4}A_{mac} \cdot$$
$$sin\,(A_{mac}))[3.66 \times 10^{-4}B_{ap} \cdot B_{mac} \cdot B_{cp} \cdot (C_{cn}-A_{cn}) \cdot cos\,(B_{cp}) + 8.3 \times$$
$$10^{-4}\frac{C_x\cdot A_{cn}\cdot A_{mac}\cdot A_{cp}^3}{A_{cp}+B_{cp}} + 6.26\Big] + 2.9\Big\} + 1.6 \times 10^{-5}\frac{B_{mac}-A_{mac}}{A_x^3} + 0.19\Big\} + 3 \times$$
$$10^{-2}\{0.973\{(0.3\sqrt{A_{cn}} - 4.7 \times 10^{-4}A_{mac} \cdot sin\,(A_{mac}))[3.66 \times 10^{-4}B_{ap} \cdot B_{mac} \cdot B_{cp} \cdot$$
$$(C_{cn}-A_{cn}) \cdot cos\,(B_{cp}) + 8.3 \times 10^{-4}\frac{C_x\cdot A_{cn}\cdot A_{mac}\cdot A_{cp}^3}{A_{cp}+B_{cp}} + 6.26\Big] + 2.9\Big\} + 1.6 \times$$

$$10^{-5}\frac{B_{mac}-A_{mac}}{A_x^3}+0.19\right\}^3\frac{1}{|B_{mac}-C_{mac}|}+2.87\right\}-1.5\times10^{-4}\frac{B_{mac}}{A_x\cdot cos\left(A_{ap}\right)}+1.08 \qquad (4)$$

5, Prediction model of τ_f for ternary materials:

$$\tau_f=1.09\frac{B_{ap}}{B_{ap}+C_{ap}}\left\{-0.33B_{en}\cdot(B_{en}-C_{en})\cdot\left\{0.75\frac{A_{ced}}{sin\left(A_{ced}\right)}\left[4.1\frac{1}{(A_v-C_v)}\cdot(-0.87\times\right.\right.$$

$$\frac{DK^3\cdot sin\left(A_v\right)\cdot sin\left(B_v\right)}{B_{mac}}+7.88\times\frac{cos\left|sin\left(\varepsilon_r\right)-sin\left(A_{cp}\right)\right|}{C_x^3}\right)+1.9\times10^{-3}\frac{B_{mac}-A_{mac}}{cos\left(B_{en}\right)}-2.27\right]+$$

$$1.89\frac{B_{ap}\cdot B_{av}^3}{A_{mac}}+3.06\right\}-0.14\right\}+4.73\times10^{-2}\frac{|A_{mac}-B_{mac}|}{A_x}\div\left(-3.57\frac{DK^3\cdot sin\left(A_v\right)\cdot sin\left(B_v\right)}{B_{mac}\cdot(A_v-C_v)}+\right.$$

$$32.3\frac{cos\left|sin\left(\varepsilon_r\right)-sin\left(A_{cp}\right)\right|}{C_x^3\cdot(A_v-C_v)}-3\times10^2\frac{1}{A_v-C_v}+1.9\times10^{-3}\frac{B_{mac}-A_{mac}}{cos\left(B_{en}\right)}-2.27\right)-2.2 \qquad (5)$$

6, Prediction model of Q_f for ternary materials:

$$Q_f=0.96\frac{B_{me}}{B_{me}+C_{me}}\left\{1.02\,cos\left(e^{-\frac{C_{mac}}{\varepsilon_r}}\right)\cdot\left\{0.36\frac{A_{cn}}{e^{A_{ir}}}[1.82C_x\cdot(A_x+C_x)(9.13\times\right.\right.$$

$$10^4\left[e^{-A_{ap}}+e^{-e^{-\frac{C_{mac}}{\varepsilon_r}}}\right]+3.55\frac{A_{cn}\cdot B_{cn}^2}{A_x\cdot A_{ir}\cdot(A_{me}+B_{me})}-6.47\times10^4\right)+3.73\times$$

$$10^4\frac{B_{aw}}{A_{mac}(B_{ym}-A_{ym})}+6.4\times10^2\right]-11.3\frac{A_{me}\cdot B_{mac}}{A_{ir}\cdot B_{cn}}+7.75\times10^3\right\}+1.04\times$$

$$10^4\,sin\left(A_{ap}\right)\cdot sin\left(B_{cn}\right)+45.1\right\}-3.69\times$$

$$10^5\frac{cos\left(9.13\times10^4\left[e^{-A_{ap}}+e^{-e^{-\frac{C_{mac}}{\varepsilon_r}}}\right]+3.55\frac{A_{cn}\cdot B_{cn}^2}{A_x\cdot A_{ir}\cdot(A_{me}+B_{me})}-6.47\times10^4\right)}{B_{me}^3}+3.64\times10^2 \qquad (6)$$

Supplementary Table 1. The associated features in these fitted models are presented in the table

Index	Notation	Feature
1	ir	Ionic radius
2	ap	Atomic polarizability
3	cp	Chemical potential
4	cn	Coordinate number
5	mac	mass attenuation coefficient for CrK_α
6	x	Normalized composition
7	ced	Core electron distance
8	v	Valence state
9	av	Atomic volume
10	aw	Atomic weight
11	ym	Young's modulus
12	me	melting enthalpy
13	en	Electronegativity