Supplementary information of Predicting Miscibility in Binary Compounds: A Machine Learning and Genetic Algorithm Study

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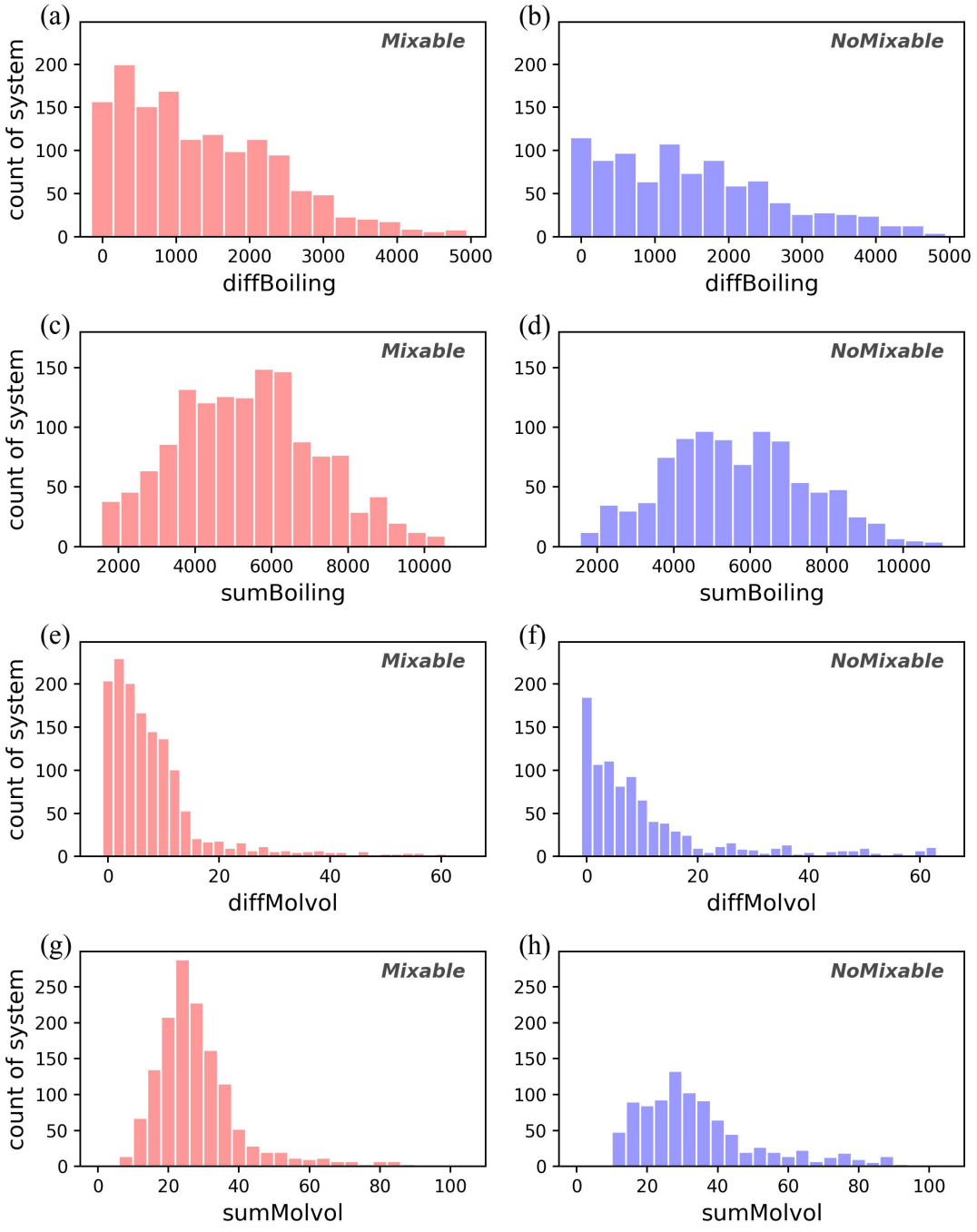
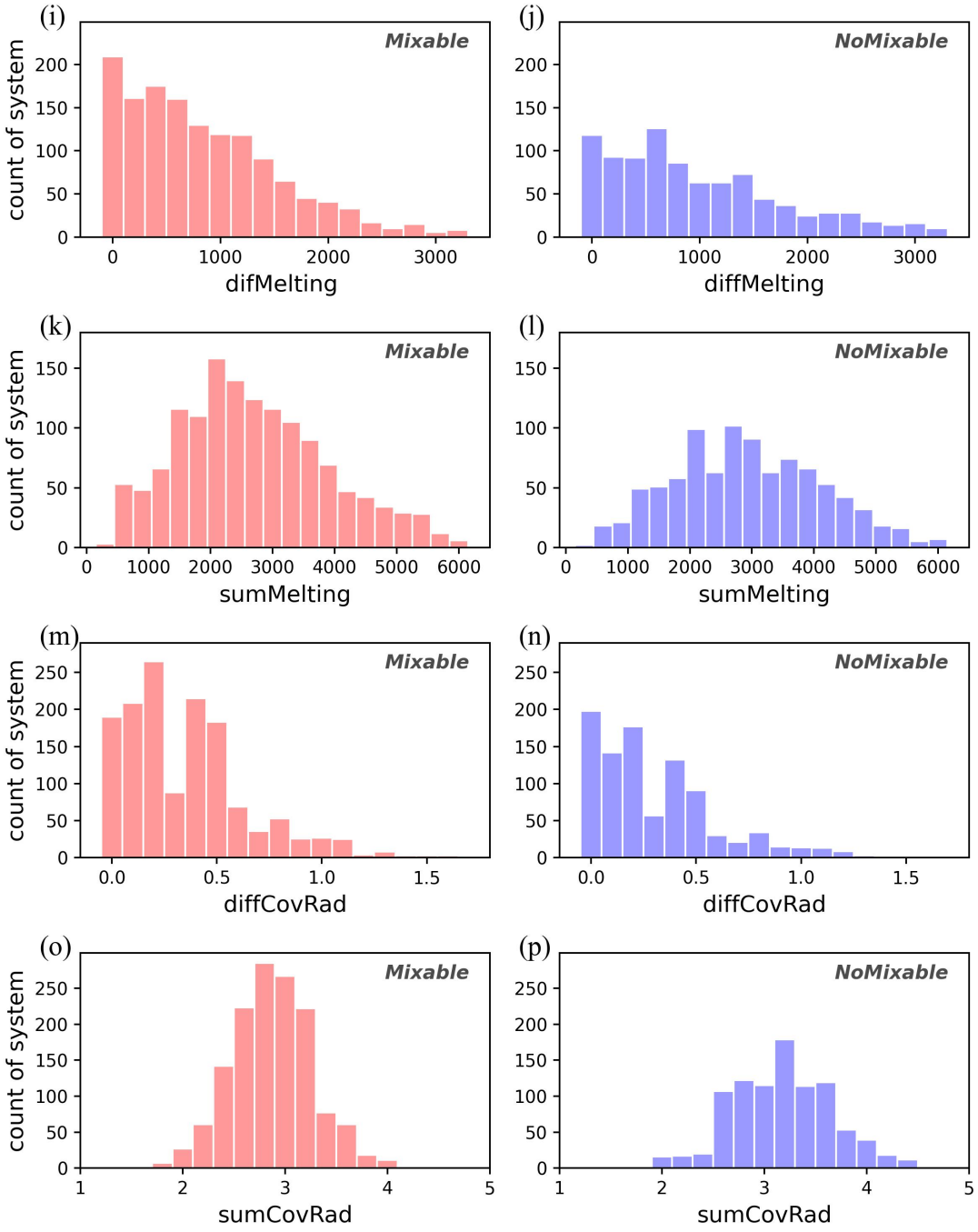

(a)
Mixable
count of system
diffBoiling
(b)
NoMixable
diffBoiling
(c)
Mixable
count of system
sumBoiling
(d)
NoMixable
sumBoiling
(e)
Mixable
count of system
diffMolvol
(f)
NoMixable
diffMolvol
(g)
Mixable
count of system
sumMolvol
(h)
NoMixable
sumMolvol


(i)
Mixable
count of system
difMelting
(j)
NoMixable
diffMelting
(k)
Mixable
sumMelting
(l)
NoMixable
sumMelting
(m)
Mixable
diffCovRad
(n)
NoMixable
diffCovRad
(o)
Mixable
sumCovRad
(p)
NoMixable
sumCovRad

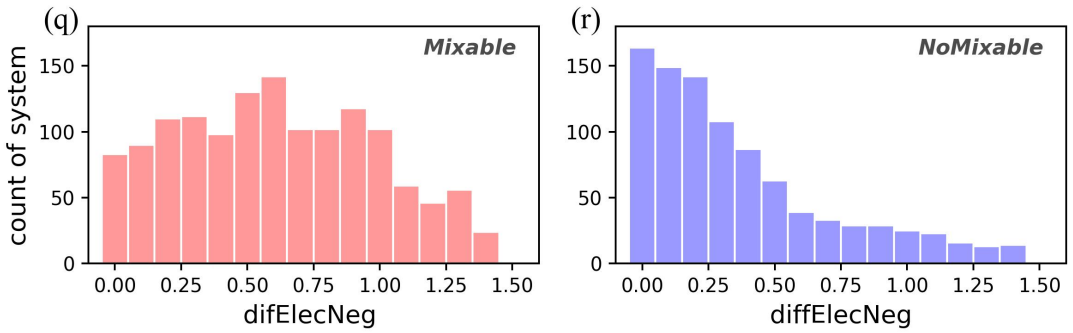


Fig. S1 Distribution of ignition point, molar volume, melting point, atomic covalent radius, and electronegativity in binary systems. The left side depicts the distribution of miscible binary systems, while the right side shows the distribution of immiscible binary systems.

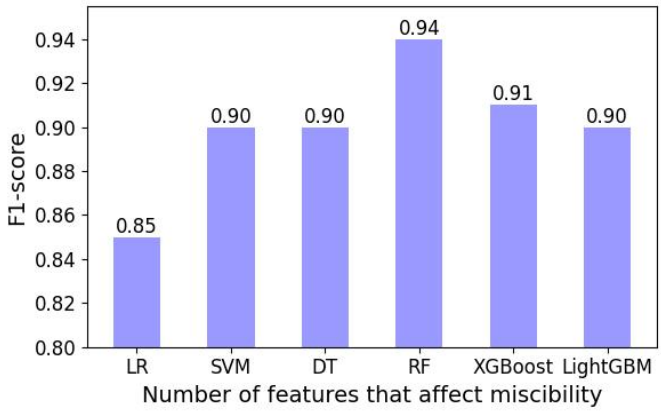


Fig. S2 Comparison of the F1-score performance of six machine learning algorithms in the task of predicting whether a binary system is miscible.

Table S3 Key hyperparameters and their setting of six algorithms.

Algorithm	Hyperparameters	Setting
LR	solver	liblinear
DT	criterion	entropy
	min_samples_split	2
SVM	C	10
RF	n_estimators	10
	criterion	entropy
	min_samples_split	2
XGBoost	n_estimators	10
LightGBM	n_estimators	10

Table S4 Partial classification results for different labels in binary systems (weighted average).

Label	Precision	Recall	F1-score	Support
diffElecNeg,sumElecNeg	0.71	0.71	0.71	470
diffCovRad,sumCovRad	0.66	0.67	0.66	470
diffMelting,sumMelting	0.56	0.55	0.56	470
diffBoiling,sumBoiling	0.61	0.61	0.61	470
diffMolVol,sumMolVol	0.68	0.67	0.68	470
sumElecNeg,sumMolVol	0.72	0.72	0.72	470
diffElecNeg,sumMolVol	0.72	0.71	0.71	470
diffElecNeg,diffMolVol	0.69	0.68	0.69	470
sumElecNeg,diffMolVol	0.73	0.73	0.73	470
sumWEle,diffWEle	0.89	0.89	0.89	470
diffElecNeg,sumElecNeg,diffUnoccupy	0.73	0.73	0.73	470
sumElecNeg,sumWEle,diffWEle	0.90	0.90	0.90	470
diffElecNeg,sumWEle,diffWEle	0.87	0.87	0.87	470
diffElecNeg,sumElecNeg,diffMolVol,sumMolVol	0.79	0.79	0.79	470
diffElecNeg,sumElecNeg,diffCovRad,sumCovRad	0.79	0.79	0.79	470
diffBoiling,sumBoiling,diffMolVol,sumMolVol	0.74	0.74	0.74	470
diffCovRad,sumCovRad,diffMelting,sumMelting	0.76	0.76	0.76	470
diffCovRad,sumCovRad,diffBoiling,sumBoiling	0.73	0.73	0.73	470
diffCovRad,sumCovRad,diffMolVol,sumMolVol	0.73	0.72	0.72	470
diffMelting,sumMelting,diffBoiling,sumBoiling	0.67	0.67	0.67	470
diffMelting,sumMelting,diffMolVol,sumMolVol	0.74	0.74	0.774	470
diffCovRad,diffMelting,diffBoiling,diffMolVol	0.70	0.70	0.70	470
sumCovRad,sumMelting,sumBoiling,sumMolVol	0.75	0.76	0.75	470
diffElecNeg,diffUnoccupy,sumWEle,diffWEle	0.90	0.89	0.89	470

sumCovRad,diffUnoccupy,sumWEle,diffWEle	0.86	0.86	0.86	470
diffCovRad,diffUnoccupy,sumWEle,diffWEle	0.88	0.87	0.87	470
sumMelting,diffUnoccupy,sumWEle,diffWEle	0.86	0.85	0.85	470
diffMelting,diffUnoccupy,sumWEle,diffWEle	0.70	0.89	0.89	470
sumMolVol,diffUnoccupy,sumWEle,diffWEle	0.89	0.88	0.88	470
diffMolVol,diffUnoccupy,sumWEle,diffWEle	0.88	0.87	0.87	470
sumBoiling,diffUnoccupy,sumWEle,diffWEle	0.88	0.88	0.88	470
diffBoiling,diffUnoccupy,sumWEle,diffWEle	0.88	0.89	0.89	470
diffBoiling,diffUnoccupy,sumWEle,diffWEle	0.88	0.89	0.89	470
diffElecNeg,sumElecNeg,diffUnoccupy,sumWEle,diffWEle	0.73	0.73	0.73	470
diffElecNeg,sumElecNeg,diffUnoccupy,diffCovRad,sumCovRad	0.79	0.79	0.79	470
diffElecNeg,sumElecNeg,diffUnoccupy,diffMolVol,sumMolVol	0.79	0.79	0.79	470
diffCovRad,sumCovRad,diffMelting,sumMelting,sumElecNeg	0.83	0.83	0.83	470
sumCovRad,sumMelting,sumBoiling,sumMolVol,sumElecNeg	0.82	0.83	0.82	470
diffCovRad,diffMelting,diffBoiling,diffMolVol,diffElecNeg	0.79	0.79	0.79	470

Table S5 Structure database of Co-Eu system.

	Phases	Symmetry	a(Å)	b(Å)	c(Å)	E_{total}(eV/atom)	E_f(meV/atom)	E_d(meV/atom)
Existing Stable Phases	Co	*Fm-3m*	3.51	3.51	3.51	-7.11	0	0
	Eu	*P6₃/mmc*	3.99	6.96	6.34	-10.26	0	0

Table S6 Crystallographic data of $CoEu_8$(space group P1).

Phases	Lattice Parameter	Wyckoff Site	Atome	x	y	z
$CoEu_8$	α=89.9969 β=89.9915 γ=111.3986 a=6.91217Å b=6.87135Å c=7.93359Å	1a	Co	-0.00291	0.49807	0.11189
		1a	Eu^1	0.24069	0.74115	0.35438
		1a	Eu^2	0.74783	0.74837	0.61301
		1a	Eu^3	0.24801	0.24774	0.61219
		1a	Eu^4	0.75453	0.25405	0.35463
		1a	Eu^5	0.75340	0.25470	0.86981
		1a	Eu^6	0.23611	0.25703	0.11167
		1a	Eu^7	0.75694	0.73764	0.11346
		1a	Eu^8	0.24024	0.74154	0.86964

Table S7 Crystallographic data of Co_3Eu_2(space group P1).

Phases	Lattice Parameter	Wyckoff Site	Atome	x	y	z
Co_3Eu_2	α=89.7127	1a	Co^1	0.67957	0.22008	0.92146
	β=60.0518	1a	Co^2	0.01326	0.17782	0.25517
	γ=89.6778	1a	Co^3	0.34695	0.13549	0.58886
	a=4.03030Å	1a	Eu^1	0.68288	0.90163	0.92416
	b=8.44895Å	1a	Eu^2	0.34442	0.45379	0.58582
	c=4.03062Å					

Table S8 Crystallographic data of CoEu(space group P1).

Phases	Lattice Parameter	Wyckoff Site	Atome	x	y	z
CoEu	α=90.0881	1a	Co^1	0.16576	0.00019	0.17525
	β=60.0075	1a	Co^2	0.83382	0.99836	0.84120
	γ=75.1617	1a	Eu^1	0.67325	0.74659	0.42052
	a=3.94870Å	1a	Eu^2	0.32599	0.25211	0.59542
	b=7.91829Å					
	c=3.94906Å					

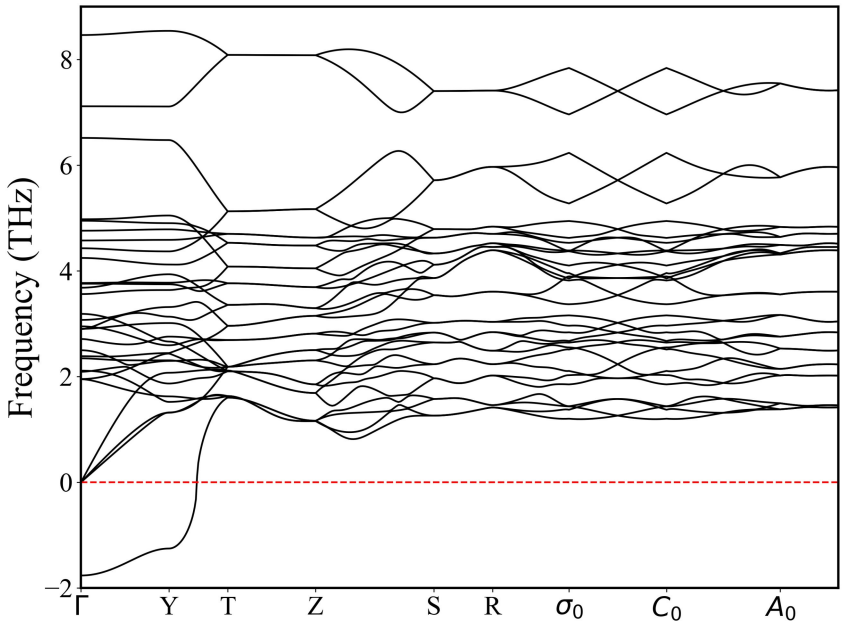


Fig. S9 Phonon band structures of Eu_2Co_3.