ADVANCED MATERIALS

Supporting Information

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Machine Learning to Predict Quasicrystals from Chemical Compositions

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Supplementary Note

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Quasicrystals and approximants used in the supervised learning

Table S1: List of quasicrystals and approximants that were used in the supervised learning. Each column gives the chemical composition, the label indicating quasicrystal or approximant (QC and AC), structure type, the known space group, and the guessed space group, respectively. The data were collected from the Crystallography of Quasicrystals handbook [1].

Composition	QC or AP	Type	Space group	Guessed space group
Cr 5 Ni 3 Si 2	QC	Octagonal		I8_4/mcm
Mn 4 Si 1	QC	Octagonal		I8_4/mcm
Mn 82 Si 15 Al 3	QC	Octagonal	I8_4/mcm	I8_4/mcm
Zn 58 Mg 40 Dy 2	QC	Decagonal		P10_5/mmc
Zn 58 Mg 40 Dy 2	QC	Decagonal		P10_5/mmc
Zn 58 Mg 40 Er 2	QC	Decagonal		P10_5/mmc
Zn 58 Mg 40 Ho 2	QC	Decagonal		P10_5/mmc
Zn 58 Mg 40 Lu 2	QC	Decagonal		P10_5/mmc
Zn 58 Mg 40 Tm 2	QC	Decagonal		P10_5/mmc
Zn 58 Mg 40 Y 2	QC	Decagonal		P10_5/mmc
Al 70 Ni 15 Fe 15	QC	Decagonal		P10_5/mmc
Al 65 Cu 15 Rh 20	QC	Decagonal		P10_5/mmc
Al 70 Ni 20 Rh 10	QC	Decagonal		P10_5/mmc
Al 65 Cu 20 Co 15	QC	Decagonal		P10_5/mmc
Al 65 Cu 20 Ir 15	QC	Decagonal		P10_5/mmc
Al 73.2 Co 26.8	AP	Decagonal	P2	P2
Al 71.5 Co 28.5	AP	Decagonal	P6_3/mmc	P6_3/mmc
Al 71.5 Co 23.6 Cu 4.9	AP	Decagonal	Cm	Cm
Al 76 Co 24	AP	Decagonal	Pmn2_1	Pmn2_1
Al 74.8 Co 17.0 Ni 8.2	AP	Decagonal	Immm	Immm
Al 71.8 Co 21.1 Ni 7.1	AP	Decagonal	Cm	Cm
Al 70.5 Mn 16.5 Pd 13	QC	Decagonal	P10_5/mmc	P10_5/mmc
Al 40 Mn 25 Fe 15 Ge 20	QC	Decagonal		P10_5/mmc
Ga 33 Fe 46 Cu 3 Si 18	QC	Decagonal		P10_5/mmc
Ga 43 Co 47 Cu 10	QC	Decagonal		P10_5/mmc
Ga 35 V 45 Ni 6 Si 14	QC	Decagonal		P10_5/mmc
Al 75 Mn 20 Pd 5	AP	Decagonal	Pnma	Pnma
Al 75 Os 10 Pd 15	QC	Decagonal	P10_5/mmc	P10_5/mmc
Al 75 Ru 10 Pd 15	QC	Decagonal		P10_5/mmc
Al 73 Ir 14.5 Os 12.5	QC	Decagonal	P10_c	P10_c
Al 70 Ni 20 Ru 10	QC	Decagonal	P10_5/mmc	P10_5/mmc
Al 72.5 Pd 27.5	AP 2/1, 1/1	Decagonal	Pna2_1	Pna2_1
Al 75 Pd 13 Ru 12	AP 3/2, 2/1	Decagonal	Pna2_1	Pna2_1
Ni 70.6 Cr 29.4	QC	Dodecagonal		P(-12)m2
V 3 Ni 2	QC	Dodecagonal		P(-12)m2
V 15 Ni 10 Si 1	QC	Dodecagonal		P(-12)m2
Ta 1.6 Te 1	QC	Dodecagonal	P(-12)m2	P(-12)m2
Ta 97 Te 60	AP	Dodecagonal	P2_12_12_1	P2_12_12_1
Ta 181 Te 112	AP	Dodecagonal	P2_12_12_1	P2_12_12_1
Al 65 Cu 20 Ru 15	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 65 Cu 20 Os 15	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 65 Cu 20 Fe 15	QC	Icosahedral	Fm-3-5	Fm-3-5

Table S1 continued

Composition	QC or AP	Type	Space group	Guessed space group
Al 70.5 Pd 21 Mn 8.5	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 70 Pd 20 Re 10	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 70 Pd 21 Tc 9	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 71 Pd 21 Re 8	QC	Icosahedral	Pm-3-5	Pm-3-5
Al 72 Pd 17 Ru 11	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 72 Pd 17 Os 11	QC	Icosahedral	Fm-3-5	Fm-3-5
Al 71.5 Cu 8.5 Ru 20	AP 1/0	Icosahedral	P2_13	P2_13
Al 55.1 Cu 14.6 Ru 20.2 Si 10.1	AP 1/0×2 (γ)	Icosahedral	Fm-3	Fm-3
Al 39 Pd 21 Fe 2	AP 1/0×2 (c)	Icosahedral	Fm-3	Fm-3
Al 68 Pd 20 Ru 12	AP 1/0×2 (c)	Icosahedral	P23	P23
Al 57.3 Cu 31.4 Ru 11.3	AP 1/1	Icosahedral	Pm-3	Pm-3
Al 55 Cu 25.5 Fe 12.5 Si 7	AP 1/1	Icosahedral	Pm-3	Pm-3
Al 40 Mn 10.1 Si 7.4	AP 1/1	Icosahedral	Pm-3	Pm-3
Al 67 Pd 11 Mn 14 Si 7	AP 1/1	Icosahedral	Pm-3	Pm-3
Al 66.6 Rh 26.1 Si 7.3	AP 2/1	Icosahedral	Pm-3	Pm-3
Al 70 Pd 23 Mn 6 Si 1	AP 2/1	Icosahedral	Pm-3	Pm-3
Zn 76 Mg 17 Hf 7	QC	Icosahedral	Fm-3-5	Fm-3-5
Zn 84 Mg 7 Zr 9	QC	Icosahedral	Pm-3-5	Pm-3-5
Al 6 Cu 1 Li 3	QC	Icosahedral	Pm-3-5	Pm-3-5
Mg 43 Al 42 Pd 15	QC	Icosahedral	Pm-3-5	Pm-3-5
Zn 40 Mg 39.5 Ga 25	QC	Icosahedral	Pm-3-5	Pm-3-5
Zn 74 Mg 15 Ho 11	QC	Icosahedral	Pm-3-5	Pm-3-5
Zn 56.8 Mg 34.6 Tb 8.7	QC	Icosahedral	Fm-3-5	Fm-3-5
Zn 65 Mg 26 Ho 9	QC	Icosahedral	Fm-3-5	Fm-3-5
Zn 64 Mg 25 Y 11	QC	Icosahedral	Fm-3-5	Fm-3-5
Zn 55 Mg 40 Nd 5	QC	Icosahedral	Pm-3-5	Pm-3-5
Zn 56.8 Mg 34.6 Dy 8.7	QC	Icosahedral	Fm-3-5	Fm-3-5
Zn 77 Mg 17.5 Ti 5.5	AP 1/1	Icosahedral	Pm-3	Pm-3
Zn 77 Mg 18 Hf 5	AP 1/1	Icosahedral	Pm-3	Pm-3
Zn 77 Mg 18 Zr 5	AP 1/1	Icosahedral	Pm-3	Pm-3
Al 88.6 Cu 19.4 Li 50.3	AP 1/1	Icosahedral	Im-3	Im-3
Zn 34.6 Mg 40 Al 25.4	AP 1/1	Icosahedral	Im-3	Im-3
Zn 61.4 Mg 24.5 Er 14.1	AP 2/1	Icosahedral	F-43m	F-43m
Zn 37 Mg 46 Al 17	AP 2/1	Icosahedral	Pm-3	Pm-3
Zn 47.3 Mg 27 Al 10.7	AP 2/1	Icosahedral	Pa-3	Pa-3
Zn 73.6 Mg 2.5 Sc 11.2	AP 2/1	Icosahedral	Pa-3	Pa-3
Zn 40 Mg 39.5 Ga 16.4 Al 4.1	AP 3/2-2/1-2/1	Icosahedral	Cmc2_1	Cmc2_1
Cu 48 Sc 15 Ga 34 Mg 3	QC	Icosahedral		Pm-3-5
Cu 46 Sc 16 Al 38	QC	Icosahedral		Pm-3-5
Zn 84 Ti 8 Mg 8	QC	Icosahedral		Pm-3-5
Zn 75 Sc 15 Ni 10	QC	Icosahedral		Pm-3-5
Zn 72 Sc 16 Cu 12	QC	Icosahedral		Pm-3-5
Zn 75 Sc 15 Co 10	QC	Icosahedral		Pm-3-5
Zn 75 Sc 15 Fe 10	QC	Icosahedral		Pm-3-5
Zn 75 Sc 15 Mn 10	QC	Icosahedral		Pm-3-5
Zn 80 Sc 15 Mg 5	QC	Icosahedral	Pm-3-5	Pm-3-5
Zn 75 Sc 15 Pt 10	QC	Icosahedral		Pm-3-5
Zn 75 Sc 15 Pd 10	QC	Icosahedral		Pm-3-5

Table S1 continued

Composition	QC or AP	Type	Space group	Guessed space group
Zn 75 Sc 15 Au 10	QC	Icosahedral		Pm-3-5
Zn 75 Sc 15 Ag 10	QC	Icosahedral		Pm-3-5
Zn 77 Sc 8 Ho 8 Fe 7	QC	Icosahedral		Pm-3-5
Zn 77 Sc 8 Er 8 Fe 7	QC	Icosahedral		Pm-3-5
Zn 77 Sc 7 Tm 9 Fe 7	QC	Icosahedral		Pm-3-5
Zn 56.8 Er 8.7 Mg 34.6	QC	Icosahedral	Fm-3-5	Fm-3-5
Zn 76 Yb 14 Mg 10	QC	Icosahedral		Fm-3-5
Cd 65 Mg 20 Lu 15	QC	Icosahedral		Fm-3-5
Ag 42 In 42 Yb 16	QC	Icosahedral	Pm-3-5	Pm-3-5
Cd 65 Mg 20 Tm 15	QC	Icosahedral		Pm-3-5
Ag 42 In 42 Ca 16	QC	Icosahedral	Pm-3-5	Pm-3-5
Au 44.2 In 41.7 Ca 14.1	QC	Icosahedral	Pm-3-5	Pm-3-5
Cd 65 Mg 20 Y 15	QC	Icosahedral	Pm-3-5	Pm-3-5
Cd 65 Mg 20 Er 15	QC	Icosahedral	Fm-3-5	Fm-3-5
Cd 65 Mg 20 Ho 15	QC	Icosahedral	Fm-3-5	Fm-3-5
Cd 65 Mg 20 Tb 15	QC	Icosahedral	Fm-3-5	Fm-3-5
Cd 65 Mg 20 Dy 15	QC	Icosahedral	Fm-3-5	Fm-3-5
Cd 65 Mg 20 Gd 15	QC	Icosahedral		Fm-3-5
Cd 84 Yb 16	QC	Icosahedral	Pm-3-5	Pm-3-5
Cd 65 Mg 20 Yb 15	QC	Icosahedral		Pm-3-5
Cd 85 Ca 15	QC	Icosahedral		Pm-3-5
Cd 65 Mg 20 Ca 15	QC	Icosahedral	Pm-3-5	Pm-3-5
Be 17 Ru 3	AP 1/1	Icosahedral		Im-3
Ga 3.85 Ni 2.15 Hf 1	AP 1/1	Icosahedral		Im-3
Ga 3.22 Ni 2.78 Zr 1	AP 1/1	Icosahedral		Im-3
Ga 3.64 Ni 2.36 Sc 1	AP 1/1	Icosahedral		Im-3
Ga 2.3 Cu 3.7 Sc 1	AP 1/1	Icosahedral		Im-3
Ga 2.6 Cu 3.4 Lu 1	AP 1/1	Icosahedral		Im-3
Zn 17 Sc 3	AP 1/1	Icosahedral		Im-3
Zn 17 Yb 3	AP 1/1	Icosahedral		Im-3
Ag 42.5 Ga 42.5 Yb 15	AP 1/1	Icosahedral		Im-3
Au 50.5 Ga 35.9 Ca 13.6	AP 1/1	Icosahedral	Im-3	Im-3
Au 61.2 Sn 23.9 Dy 15.2	AP 1/1	Icosahedral		Im-3
Au 62.3 Sn 23.1 Gd 14.6	AP 1/1	Icosahedral		Im-3
Ag 42.2 In 42.6 Tm 15.2	AP 1/1	Icosahedral		Im-3
Au 47.2 In 37.2 Gd 15.6	AP 1/1	Icosahedral		Im-3
Au 12.2 In 6.3 Ca 3	AP 1/1	Icosahedral	Im-3	Im-3
Au 64.2 Sn 21.3 Pr 14.5	AP 1/1	Icosahedral		Im-3
Au 65 Sn 20 Ce 15	AP 1/1	Icosahedral	Im-3	Im-3
Ag 46.4 In 39.7 Gd 13.9	AP 1/1	Icosahedral		Im-3
Au 49.7 In 35.4 Ce 14.9	AP 1/1	Icosahedral		Im-3
Au 60.7 Sn 25.2 Eu 14.1	AP 1/1	Icosahedral		Im-3
Ag 2 In 4 Yb 1	AP 1/1	Icosahedral	Im-3	Im-3
Ag 46.9 In 38.7 Pr 14.4	AP 1/1	Icosahedral		Im-3
Au 42 In 42 Yb 16	AP 1/1	Icosahedral	Ia-3	Ia-3
Cd 6 Gd 1	AP 1/1	Icosahedral	Im-3	Im-3
Ag 2 In 4 Ca 1	AP 1/1	Icosahedral	Im-3	Im-3
Ag 47.7 In 38.7 Ce 14.2	AP 1/1	Icosahedral		Im-3

Table S1 continued

Composition	QC or AP	Type	Space group	Guessed space group
Cd 6 Dy 1	AP 1/1	Icosahedral	Im-3	Im-3
Cd 6 Y 1	AP 1/1	Icosahedral		Im-3
Cd 6 Sm 1	AP 1/1	Icosahedral	Im-3	Im-3
Cd 6 Nd 1	AP 1/1	Icosahedral	Im-3	Im-3
Cd 6 Yb 1	AP 1/1	Icosahedral	Im-3	Im-3
Ag 42.9 In 43.6 Eu 13.5	AP 1/1	Icosahedral		Im-3
Cd 6 Ca 1	AP 1/1	Icosahedral	Im-3	Im-3
Cd 25 Eu 4	AP 1/1×2	Icosahedral	Fd-3	Fd-3
Cd 19 Pr 3	AP 1/1	Icosahedral	Im-3	Im-3
Cd 6 Sr 1	AP 1/1	Icosahedral		Im-3
Au 61.1 Ga 25.0 Ca 13.9	AP 2/1	Icosahedral	Pa-3	Pa-3
Au 60.3 Sn 24.6 Yb 15.1	AP 2/1	Icosahedral		Pa-3
Au 61.2 Sn 24.3 Ca 14.5	AP 2/1	Icosahedral		Pa-3
Au 42.9 In 41.9 Yb 15.2	AP 2/1	Icosahedral	Pa-3	Pa-3
Au 37 In 39.6 Ca 12.6	AP 2/1	Icosahedral	Pa-3	Pa-3
Ag 41.7 In 43.2 Yb 15.1	AP 2/1	Icosahedral	Pa-3	Pa-3
Au 61.2 Sn 24.5 Eu 14.3	AP 2/1	Icosahedral		Pa-3
Ag 41 In 44 Yb 15	AP 2/1	Icosahedral		Pa-3
Ag 42 In 45 Ca 13	AP 2/1	Icosahedral	Pa-3	Pa-3
Cd 76 Ca 13	AP 2/1	Icosahedral	Pa-3	Pa-3
Ag 43.4 In 42.8 Eu 13.8	AP 2/1	Icosahedral	Pa-3	Pa-3

Element features

Table S2: 58 element features that were used to calculate the compositional descriptors. The dataset is accessible at our open-source software XenonPy [2].

Feature ID	Description	Unit	Reference
atomic_number	Atomic number		
atomic_radius	Atomic radius	pm	[3, 4]
atomic_radius_rahm	Atomic radius by Rahm et al.	pm	[4–6]
atomic_volume	Atomic volume	$cm^3\ mol^{-1}$	[4]
atomic_weight	Atomic weight		[4, 7, 8]
boiling_point	Boiling temperature	K	[4]
bulk_modulus	Bulk modulus	GPa	[9]
c6_gb	C_6 dispersion coefficient in a.u. (Gould & Bučko)	a.u.	[4, 10, 11]
covalent_radius_cordero	Covalent radius by Cerdero et al.	pm	[4, 12]
covalent_radius_pyykko	Single bond covalent radius by Pyykko et al.	pm	[4, 13]
covalent_radius_pyykko_double	Double bond covalent radius by Pyykko et al.	pm	[4, 14]
covalent_radius_pyykko_triple	Triple bond covalent radius by Pyykko et al.	pm	[4, 15]
covalent_radius_slater	Covalent radius by Slater	pm	[3]
density	Density at 295K	$g\ cm^3$	[4]
dipole_polarizability	Dipole polarizability	a.u,	[4, 16]
electron_negativity	Pauling electronegativity		[17]
electron_affinity	Electron affinity	eV	[4, 18, 19]
en_allen	Allen's scale of electronegativity	eV	[4, 20, 21]
en_ghosh	Ghosh's scale of electronegativity		[4, 22]
en_pauling	Pauling's scale of electronegativity		[4, 18]
first_ion_en	First ionization energy	eV	[18]
fusion_enthalpy	Enthalpy of fusion for elements at their melting temperatures	$kJ\ mol^{-1}$	[18]
gs_bandgap	DFT bandgap energy of T=0K ground state	eV	[23, 24]
gs_energy	DFT energy per atom (raw VASP value) of T=0K ground state	$eV\ atom^{-1}$	[23, 24]
gs_est_bcc_latcnt	Estimated BCC lattice parameter based on the DFT volume of the OQMD ground state for each element		[23, 24]
gs_est_fcc_latcnt	Estimated FCC lattice parameter based on the DFT volume of the OQMD ground state for each element	Å	[23, 24]
gs_mag_moment	DFT magnetic moment of T=0K ground state		[23, 24]
gs_volume_per	DFT volume per atom of T=0K ground state	$Å^3\ atom^{-1}$	[23, 24]
hhi_p	HerfindahlHirschman Index (HHI) production values		[25]
hhi_r	HerfindahlHirschman Index (HHI) reserves values		[25]

Table S2 continued

Feature ID	Description	Unit	Reference
heat_capacity_mass	Specific heat capacity at STP[1]	J mol^{-1} K^{-1}	[18]
heat_capacity_molar	Molar heat capacity at STP	J mol^{-1} K^{-1}	[18]
icsd_volume	Volume per atom of ICSD phae at STP		[26–28]
evaporation_heat	Evaporation heat	kJ mol^{-1}	[4]
heat_of_formation	Heat of formation	kJ mol^{-1}	[4]
lattice_constant	Lattice constant	Å	[4]
mendeleev_number	Mendeleev's number		[4, 29, 30]
melting_point	Melting temperature	K	[4]
molar_volume	Molar volume	L mol^{-1}	[9]
num_unfilled	Number of unfilled valence orbitals		[31, 32]
num_valance	Number of valence electrons		[31, 32]
num_d_unfilled	Number of unfilled d valence orbitals		[31, 32]
num_d_valence	Number of filled d valence orbitals		[31, 32]
num_f_unfilled	Number of unfilled f valence orbitals		[31, 32]
num_f_valence	Number of filled f valence orbitals		[31, 32]
num_p_unfilled	Number of unfilled p valence orbitals		[31, 32]
num_p_valence	Number of filled p valence orbitals		[31, 32]
num_s_unfilled	Number of unfilled s valence orbitals		[31, 32]
num_s_valence	Number of filled s valence orbitals		[31, 32]
period	Period in periodic table		[4]
specific_heat	Specific heat at 20 °C	J g^{-1} mol^{-1}	[4]
thermal_conductivity	Thermal conductivity at 25 °C	W m^{-1} K^{-1}	[4]
vdw_radius	van der Waals radius	pm	[4, 18]
vdw_radius_alvarez	van der Waals radius according to Alvarez	pm	[4, 33]
vdw_radius_mm3	van der Waals radius from the MM3 FF	pm	[4, 34]
vdw_radius_uff	van der Waals radius from the UFF	pm	[4, 35]
sound_velocity	Velocity of sound	m s^{-1}	[9]
polarizability	Static average electric dipole polarizability	$10^{-24}cm^3$	[18]

[1]Standard Temperature and Pressure

Generalization ability of the model

Table S3: Prediction performance for the three-class classification problem of stable quasicrystals (QC), approximants (AC), and others. The left table is the confusion matrix, and the right table reports the per-class recall, precision, and F_1 metrics. The performance metrics were averaged over 100 different bootstrap sets, and the numbers in parentheses represent the standard deviations. The results labeled as "with Al systems" are the same as we report in Table 1. Additionally, in the "without Al systems" panel, we show the results of the performance evaluation after eliminating the aluminum-containing compositions from the test instances.

			Predicted class		
Test set			QC	AC	others
With Al systems	True class	QC	9.63 (1.641)	3.24 (1.342)	3.13 (1.189)
		AC	3.11 (1.555)	9.73 (1.805)	3.16 (1.573)
		others	0.76 (0.896)	0.42 (0.619)	2016.82 (1.024)
Without Al systems	True class	QC	7.14 (1.594)	1.91 (1.150)	1.90 (1.221)
		AC	1.43 (1.185)	7.68 (1.788)	2.36 (1.389)
		others	0.45 (0.698)	0.16 (0.367)	1900.13 (8.795)

Performance metrics			
	Recall	Precision	F_1
QC	0.602 (0.103)	0.722 (0.090)	0.650 (0.076)
AC	0.608 (0.113)	0.731 (0.089)	0.658 (0.088)
others	0.999 (0.001)	0.997 (0.001)	0.998 (0.001)
QC	0.662 (0.140)	0.807 (0.125)	0.715 (0.102)
AC	0.671 (0.137)	0.792 (0.110)	0.720 (0.108)
others	1.000 (0.000)	0.998 (0.001)	0.999 (0.001)

Prediction accuracy sensitivity

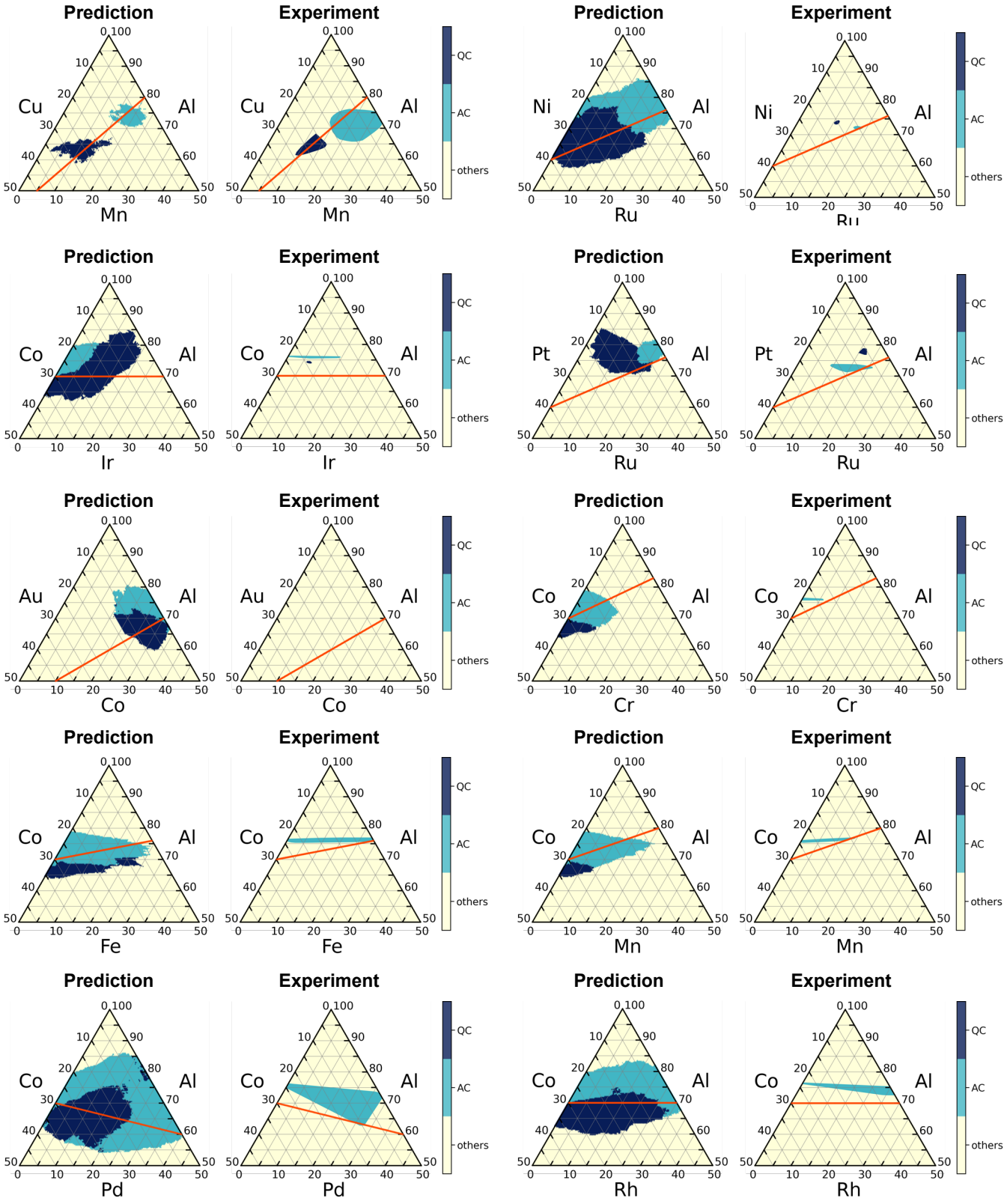
Table S4: The sensitivity of the prediction accuracy when using the different sample sizes of periodic crystals ($N_{crystal}$). The left table is the confusion matrix, and the right table reports the per-class recall, precision, and F_1 metrics. The performance metrics were averaged over 100 different bootstrap sets, and the numbers in parentheses represent the standard deviations.

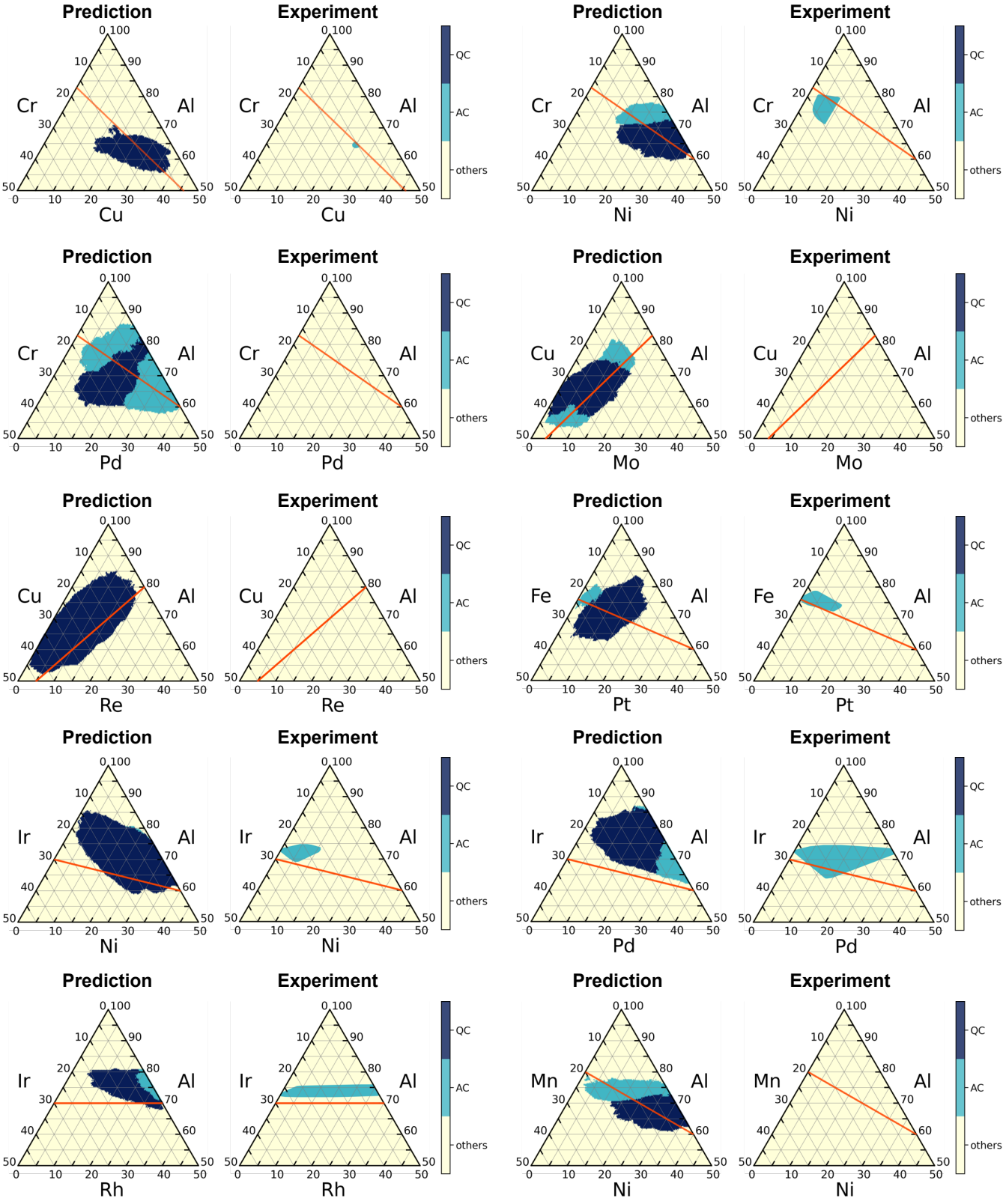
		Predicted class		
$N_{crystal}$	True class	QC	AC	others
500	QC	11.08 (2.58)	3.58 (1.97)	0.88 (1.04)
	AC	3.48 (1.75)	10.75 (2.98)	1.13 (1.12)
	others	0.61 (0.84)	0.35 (0.64)	118.14 (4.25)
2,500	QC	9.90 (3.10)	3.65 (1.80)	2.19 (1.44)
	AC	3.48 (1.82)	9.88 (2.59)	2.03 (1.38)
	others	0.38 (0.61)	0.49 (0.67)	518.00 (4.82)
5,000	QC	9.96 (2.83)	3.47 (1.77)	2.40 (1.41)
	AC	2.95 (1.81)	9.67 (2.75)	2.84 (1.68)
	others	0.37 (0.67)	0.66 (0.78)	1017.68 (4.86)
10,000	QC	9.73 (2.75)	3.17 (1.62)	3.02 (1.68)
	AC	2.68 (1.70)	8.54 (2.33)	3.67 (1.98)
	others	0.50 (0.70)	0.72 (0.83)	2017.97 (5.19)
15,000	QC	9.47 (2.94)	3.33 (2.04)	3.49 (1.58)
	AC	2.90 (1.66)	8.46 (2.22)	4.65 (2.44)
	others	0.49 (0.69)	1.18 (1.03)	3016.03 (4.84)
20,000	QC	9.39 (2.69)	2.85 (1.89)	3.92 (2.12)
	AC	2.74 (1.68)	8.80 (2.68)	4.78 (2.53)
	others	0.64 (0.83)	1.26 (1.08)	4015.62 (5.11)
25,000	QC	9.29 (2.68)	2.64 (1.57)	3.83 (1.77)
	AC	2.84 (1.77)	7.70 (2.27)	5.75 (2.51)
	others	0.71 (0.85)	1.16 (1.08)	5016.08 (4.96)
30,000	QC	9.45 (2.77)	2.65 (1.61)	4.20 (1.83)
	AC	2.32 (1.39)	7.37 (2.30)	5.66 (2.47)
	others	0.83 (0.93)	1.45 (1.19)	6016.07 (4.79)

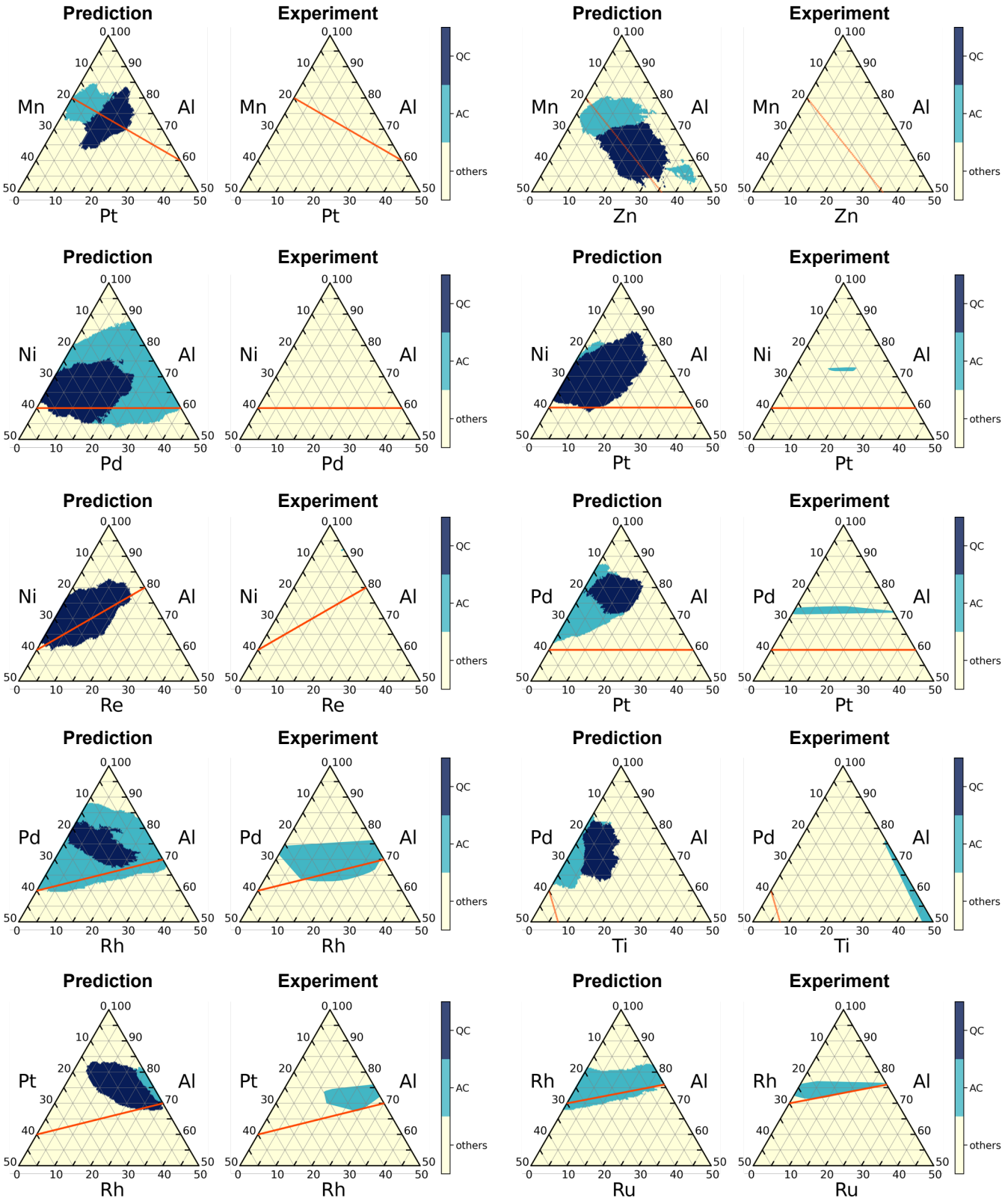
	Performance metrics		
	Recall	Precision	F_1
QC	0.719 (0.121)	0.736 (0.107)	0.719 (0.086)
AC	0.701 (0.125)	0.735 (0.127)	0.708 (0.096)
others	0.992 (0.009)	0.983 (0.012)	0.988 (0.007)
QC	0.627 (0.132)	0.718 (0.120)	0.661 (0.109)
AC	0.645 (0.120)	0.708 (0.107)	0.668 (0.093)
others	0.998 (0.002)	0.992 (0.004)	0.995 (0.002)
QC	0.627 (0.123)	0.756 (0.128)	0.677 (0.102)
AC	0.631 (0.124)	0.704 (0.120)	0.655 (0.096)
others	0.999 (0.001)	0.995 (0.002)	0.997 (0.001)
QC	0.609 (0.135)	0.758 (0.127)	0.666 (0.112)
AC	0.584 (0.127)	0.694 (0.112)	0.623 (0.091)
others	0.999 (0.001)	0.997 (0.001)	0.998 (0.001)
QC	0.582 (0.133)	0.736 (0.113)	0.641 (0.105)
AC	0.536 (0.123)	0.663 (0.127)	0.581 (0.098)
others	0.999 (0.000)	0.997 (0.001)	0.998 (0.001)
QC	0.585 (0.128)	0.739 (0.118)	0.643 (0.101)
AC	0.548 (0.133)	0.688 (0.136)	0.597 (0.107)
others	1.000 (0.000)	0.998 (0.001)	0.999 (0.000)
QC	0.593 (0.122)	0.728 (0.138)	0.644 (0.107)
AC	0.479 (0.129)	0.677 (0.133)	0.550 (0.116)
others	1.000 (0.000)	0.998 (0.001)	0.999 (0.000)
QC	0.583 (0.123)	0.750 (0.117)	0.648 (0.102)
AC	0.483 (0.122)	0.642 (0.145)	0.542 (0.113)
others	1.000 (0.000)	0.998 (0.000)	0.999 (0.000)

Phase diagram

Figure S1: Predicted and experimentally determined phase diagrams for the 30 Al-TM-TM alloy systems. For each system, the left panel shows the predicted diagram made by the random forest classifier, and the right panel shows the actual phase diagram extracted from the literature. Three different colors are used to distinguish the phase region of quasicrystals, approximants, and others.

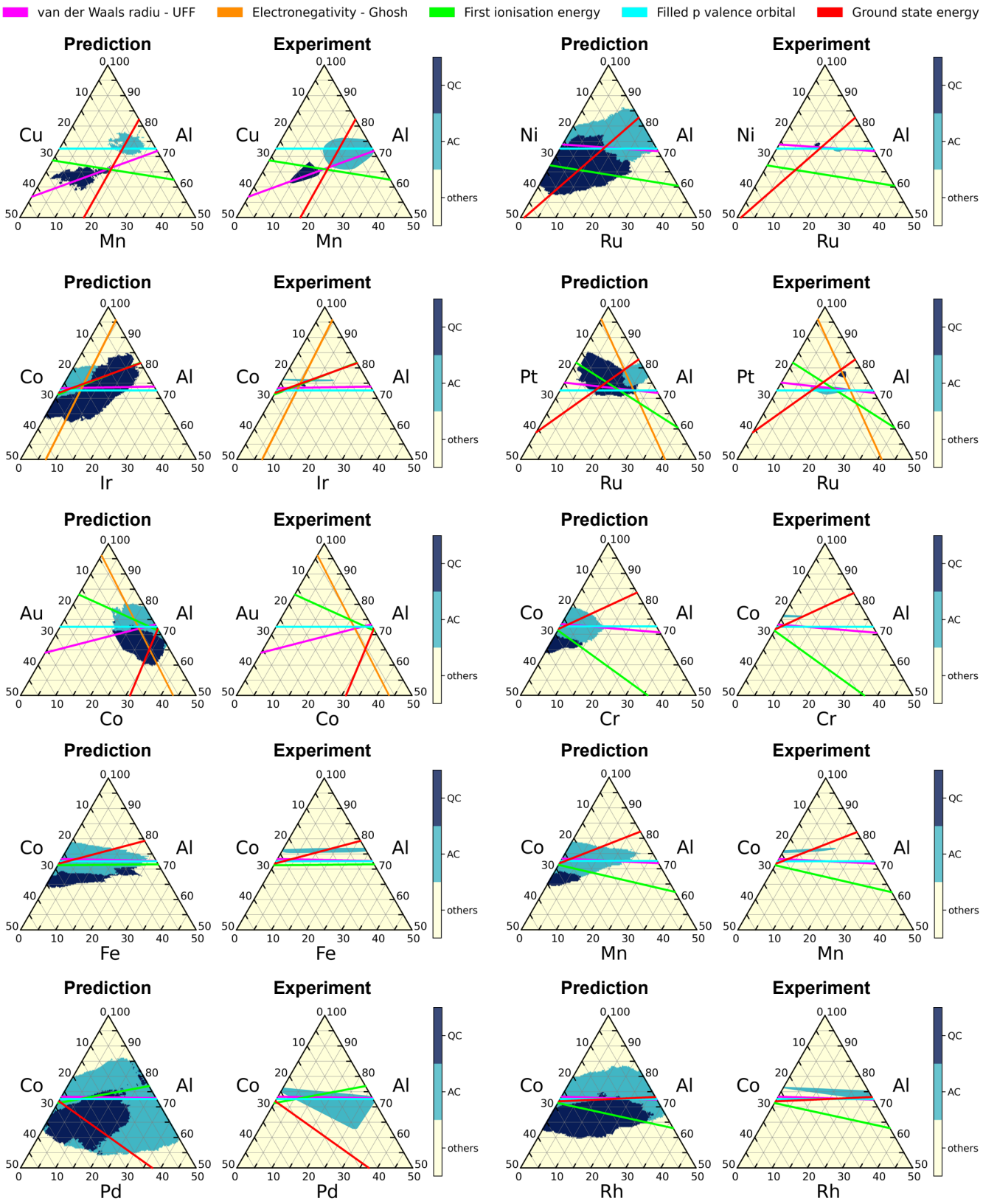


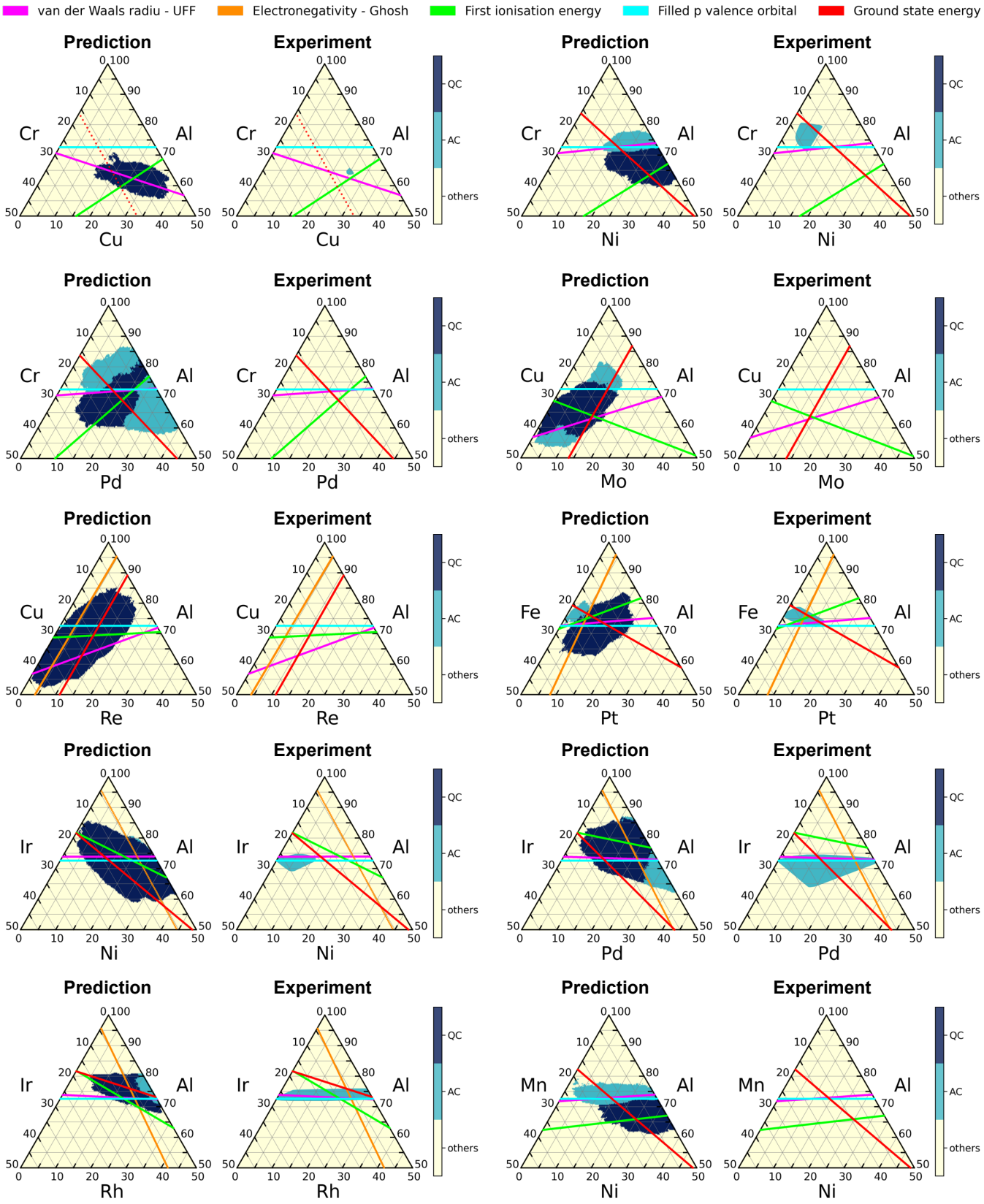

Prediction
Experiment
Cr
Al
Cu
Ni
Pd
Mo
Re
Fe
Pt
Ir
Rh
Mn
QC
AC
others

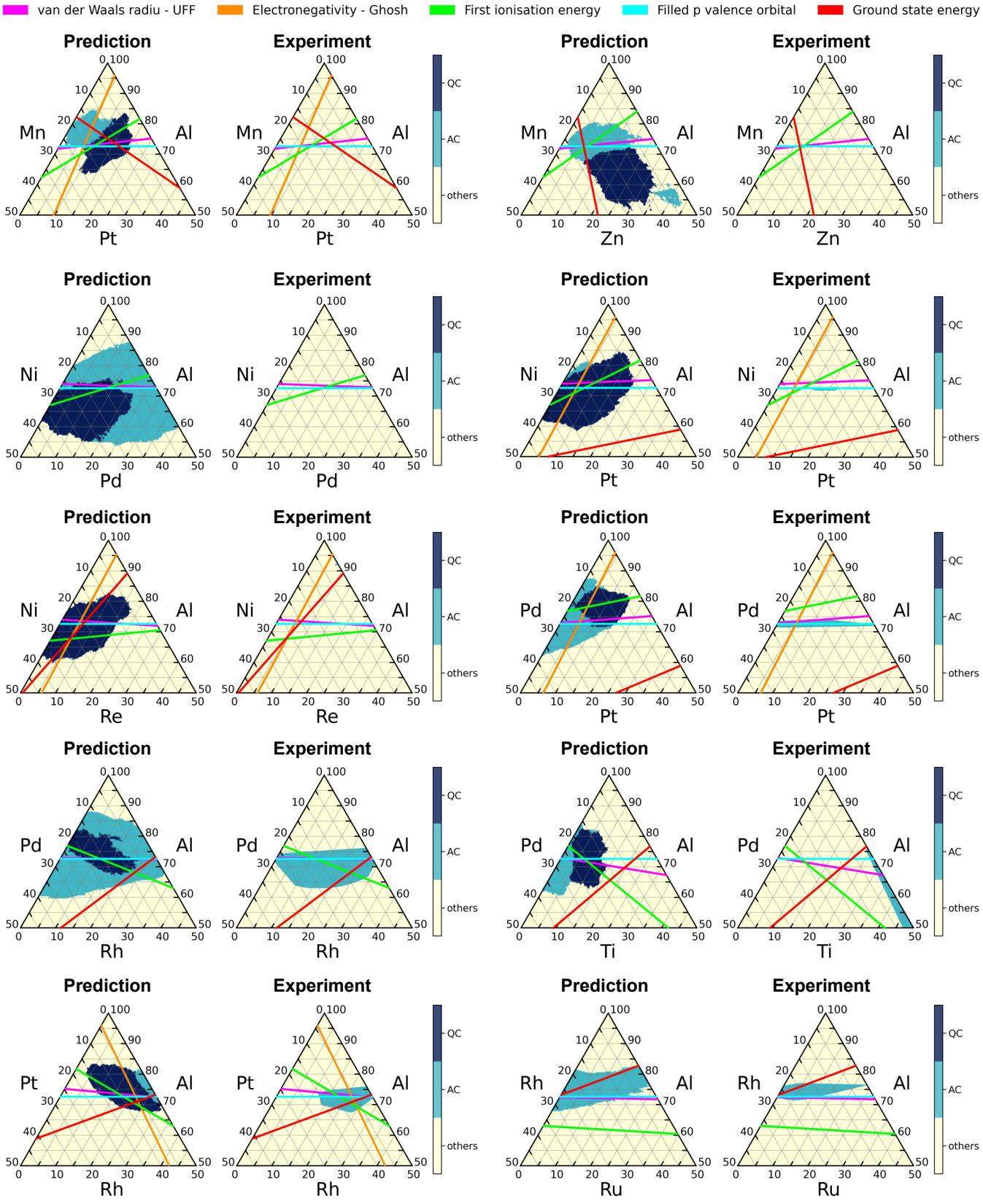

Prediction
Experiment
Mn
Al
Pt
Zn
Ni
Pd
Re
Rh
Ti
Ru
QC
AC
others

Machine learning learned rules

Figure S2: The formation rules of QC/AC discovered by the machine learning algorithm are overwritten on the predicted phase diagrams of the 30 Al-TM-TM systems. A color-coded line represents a condition imposed on the weighted average of van der Waals radius, electronegativity, first ionisation energy, the number of filled p valence orbitals, or the energy per atom at T=0K ground state.




van der Waals radiu - UFF
Electronegativity - Ghosh
First ionisation energy
Filled p valence orbital
Ground state energy
Prediction
Experiment
Cr Al Cu
Cr Al Ni
Cr Al Pd
Cu Al Mo
Cu Al Re
Fe Al Pt
Ir Al Ni
Ir Al Pd
Ir Al Rh
Mn Al Ni
QC
AC
others


van der Waals radiu - UFF
Electronegativity - Ghosh
First ionisation energy
Filled p valence orbital
Ground state energy
Prediction
Experiment
Mn
Al
Pt
Zn
Ni
Pd
Re
Pd
Rh
Ti
Pt
Rh
Rh
Ru
QC
AC
others

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