

# Composition engineering on the local structure and viscosity of the steelmaking slag by machine learning methods

**Table S1.** Component content of different converter slag systems.

Model	P <sub>2</sub> O <sub>5</sub> /wt %	CaO/wt %	SiO <sub>2</sub> /wt %	FeO/wt %	Density/(g/cm <sup>3</sup> )
P1	1	41.4	27.6	30	3.104752
P2	2	40.8	27.2	30	3.091227
P3	3	40.2	26.8	30	3.077814
P4	4	39.6	26.4	30	3.064512
P5	5	39	26	30	3.05132
P6	6	38.4	25.6	30	3.038235
P7	7	37.8	25.2	30	3.025258
P8	8	37.2	24.8	30	3.012386
P9	9	36.6	24.4	30	2.999619
P10	10	36	24	30	2.986954
P11	15	33	22	30	2.925134
P12	20	30	20	30	2.865711
P13	25	27	18	30	2.808548
P14	30	24	16	30	2.753519

Model	Al <sub>2</sub> O <sub>3</sub> /wt %	CaO/wt %	SiO <sub>2</sub> /wt %	FeO/wt %	Density/( g/cm <sup>3</sup> )
A1	1	41.4	27.6	30	2.874681
A2	2	40.8	27.2	30	2.870054
A3	3	40.2	26.8	30	2.86544
A4	4	39.6	26.4	30	2.86084
A5	5	39	26	30	2.856255
A6	6	38.4	25.6	30	2.851683
A7	7	37.8	25.2	30	2.847125
A8	8	37.2	24.8	30	2.842582
A9	9	36.6	24.4	30	2.838052
A10	10	36	24	30	2.833536
A11	15	33	22	30	2.811158
A12	20	30	20	30	2.789115
A13	25	27	18	30	2.767399
A14	30	24	16	30	2.746003

Model	P <sub>2</sub> O <sub>5</sub> /wt %	Al <sub>2</sub> O <sub>3</sub> /wt %	CaO/wt %	SiO <sub>2</sub> /wt %	FeO/wt %	Density/(g/cm <sup>3</sup> )
A2P2	2	2	39.6	26.4	30	3.080612
A2P4	2	4	38.4	25.6	30	3.070067
A2P6	2	6	37.2	24.8	30	3.05959
A2P8	2	8	36	24	30	3.049182
A2P10	2	10	34.8	23.2	30	3.038842
A2P12	2	12	33.6	22.4	30	3.028568
A4P2	4	2	38.4	25.6	30	3.054072
A4P4	4	4	37.2	24.8	30	3.043699
A4P6	4	6	36	24	30	3.033394
A4P8	4	8	34.8	23.2	30	3.023156
A4P10	4	10	33.6	22.4	30	3.012983
A4P12	4	12	32.4	21.6	30	3.002875

A6P2	6	2	37.2	24.8	30	3.027966
A6P4	6	4	36	24	30	3.017762
A6P6	6	6	34.8	23.2	30	3.007624
A6P8	6	8	33.6	22.4	30	2.99755
A6P10	6	10	32.4	21.6	30	2.987541
A6P12	6	12	31.2	20.8	30	2.977596
A8P2	8	2	36	24	30	3.002283
A8P4	8	4	34.8	23.2	30	2.992243
A8P6	8	6	33.6	22.4	30	2.982268
A8P8	8	8	32.4	21.6	30	2.972356
A8P10	8	10	31.2	20.8	30	2.962507
A8P12	8	12	30	20	30	2.95272
A10P2	10	2	34.8	23.2	30	2.977013
A10P4	10	4	33.6	22.4	30	2.967134
A10P6	10	6	32.4	21.6	30	2.957318
A10P8	10	8	31.2	20.8	30	2.947563
A10P10	10	10	30	20	30	2.93787
A10P12	10	12	28.8	19.2	30	2.928238
A12P2	12	2	33.6	22.4	30	2.952146
A12P4	12	4	32.4	21.6	30	2.942424
A12P6	12	6	31.2	20.8	30	2.932763
A12P8	12	8	30	20	30	2.923162
A12P10	12	10	28.8	19.2	30	2.913622
A12P12	12	12	27.6	18.4	30	2.90414

**Table S2.** Bond lengths of major atom pairs for different models.

Model	Si-O/(rdf-1)Å	Ca-O/(rdf-1)Å	Fe-O/(rdf-1)Å	P-O/(rdf-1)Å	Al-O/(rdf-1)Å
Exp	1.61-1.62 [1,2]	2.29-2.83 [1,2]	2.05-2.09 [1,2]	1.53 [1]	1.72-1.76 [2]
P1	1.619	2.340	2.079	1.533	--
P2	1.619	2.342	2.079	1.548	--
P3	1.619	2.342	2.089	1.533	--
P4	1.619	2.342	2.079	1.548	--
P5	1.619	2.342	2.071	1.533	--
P6	1.619	2.340	2.079	1.533	--
P7	1.619	2.342	2.071	1.533	--
P8	1.619	2.342	2.089	1.533	--
P9	1.619	2.342	2.089	1.533	--
P10	1.619	2.342	2.076	1.548	--
P11	1.619	2.340	2.079	1.533	--
P12	1.619	2.342	2.089	1.533	--
P13	1.619	2.342	2.089	1.534	--
P14	1.619	2.348	2.089	1.534	--
A1	1.619	2.342	2.057	--	1.752
A2	1.619	2.342	2.071	--	1.748
A3	1.619	2.342	2.057	--	1.748
A4	1.619	2.342	2.046	--	1.748
A5	1.619	2.342	2.057	--	1.748
A6	1.619	2.342	2.057	--	1.748
A7	1.619	2.342	2.071	--	1.748
A8	1.619	2.342	2.071	--	1.748
A9	1.619	2.342	2.071	--	1.748
A10	1.619	2.342	2.057	--	1.748

A11	1.619	2.342	2.071	--	1.748
A12	1.619	2.341	2.046	--	1.748
A13	1.619	2.342	2.071	--	1.748
A14	1.619	2.342	2.046	--	1.748
A2P2	1.619	2.342	2.077	1.526	1.752
A2P4	1.619	2.342	2.075	1.548	1.752
A2P6	1.619	2.342	2.071	1.538	1.752
A2P8	1.619	2.342	2.073	1.548	1.752
A2P10	1.619	2.342	2.073	1.538	1.752
A2P12	1.619	2.342	2.079	1.538	1.752
A4P2	1.619	2.342	2.079	1.538	1.752
A4P4	1.619	2.342	2.082	1.538	1.752
A4P6	1.619	2.342	2.071	1.541	1.752
A4P8	1.619	2.342	2.082	1.538	1.756
A4P10	1.619	2.342	2.079	1.541	1.756
A4P12	1.619	2.342	2.082	1.538	1.752
A6P2	1.619	2.342	2.079	1.538	1.756
A6P4	1.619	2.342	2.085	1.538	1.752
A6P6	1.619	2.342	2.079	1.538	1.752
A6P8	1.619	2.342	2.085	1.538	1.752
A6P10	1.619	2.342	2.079	1.538	1.756
A6P12	1.619	2.342	2.079	1.538	1.752
A8P2	1.619	2.342	2.085	1.538	1.752
A8P4	1.619	2.342	2.085	1.545	1.752
A8P6	1.619	2.342	2.085	1.540	1.752
A8P8	1.619	2.342	2.085	1.554	1.752
A8P10	1.619	2.342	2.079	1.538	1.752
A8P12	1.619	2.342	2.079	1.538	1.752
A10P2	1.619	2.342	2.079	1.549	1.752
A10P4	1.619	2.342	2.079	1.549	1.752
A10P6	1.619	2.342	2.079	1.549	1.752
A10P8	1.619	2.342	2.079	1.549	1.752
A10P10	1.619	2.342	2.079	1.538	1.752
A10P12	1.619	2.342	2.079	1.538	1.752
A12P2	1.619	2.342	2.077	1.549	1.752
A12P4	1.619	2.342	2.077	1.541	1.752
A12P6	1.619	2.342	2.086	1.538	1.752
A12P8	1.619	2.342	2.081	1.535	1.752
A12P10	1.619	2.342	2.081	1.538	1.752
A12P12	1.619	2.342	2.081	1.538	1.752

**Table S3.** The coordination number of each major atomic pair for different models.

P-O									
P1	3.998016	A1	--	A2P2	3.998006	A6P2	3.998014	A10P2	3.998038
P2	3.998014	A2	--	A2P4	3.998031	A6P4	3.99802	A10P4	3.998031
P3	3.99801	A3	--	A2P6	3.998019	A6P6	3.998025	A10P6	3.998015
P4	3.998029	A4	--	A2P8	3.998027	A6P8	3.9946	A10P8	3.998037
P5	3.998012	A5	--	A2P10	3.998024	A6P10	3.998016	A10P10	3.998023
P6	3.989096	A6	--	A2P12	3.998018	A6P12	3.99573	A10P12	3.99803
P7	3.998026	A7	--	A4P2	3.998009	A8P2	3.998012	A12P2	3.998039
P8	3.99803	A8	--	A4P4	3.991271	A8P4	3.998025	A12P4	3.998036
P9	3.998022	A9	--	A4P6	3.993484	A8P6	3.993481	A12P6	3.993472

P10	3.998026	A10	— —	A4P8	3.998026	A8P8	3.994608	A12P8	3.998024
P11	3.998022	A11	— —	A4P10	3.998017	A8P10	3.998024	A12P10	3.998029
P12	3.99802	A12	— —	A4P12	3.998023	A8P12	3.995729	A12P12	3.995711
P13	3.995791	A13	— —						
P14	3.996149	A14	— —						

#### Al-O

P1	— —	A1	4.056149	A2P2	4.065755	A6P2	4.133048	A10P2	4.123436
P2	— —	A2	4.017678	A2P4	4.008079	A6P4	4.118564	A10P4	4.119534
P3	— —	A3	4.075356	A2P6	4.113806	A6P6	4.06987	A10P6	4.122446
P4	— —	A4	4.041707	A2P8	4.094597	A6P8	4.105575	A10P8	4.094892
P5	— —	A5	4.06766	A2P10	4.075359	A6P10	4.116861	A10P10	4.091697
P6	— —	A6	4.036907	A2P12	4.094594	A6P12	4.123431	A10P12	4.093679
P7	— —	A7	4.058879	A4P2	4.137846	A8P2	4.09553	A12P2	4.122623
P8	— —	A8	4.039708	A4P4	4.118624	A8P4	4.136786	A12P4	4.140592
P9	— —	A9	4.04802	A4P6	4.125877	A8P6	4.11363	A12P6	4.125082
P10	— —	A10	4.064328	A4P8	4.165092	A8P8	4.103829	A12P8	4.150746
P11	— —	A11	4.029867	A4P10	4.101386	A8P10	4.119727	A12P10	4.081224
P12	— —	A12	4.04607	A4P12	4.06707	A8P12	4.124671	A12P12	4.081779
P13	— —	A13	4.041718						
P14	— —	A14	4.053035						

#### Si-O

P1	4.007113	A1	3.998174	A2P2	4.005877	A6P2	4.006433	A10P2	4.00412
P2	3.999831	A2	3.998178	A2P4	3.999948	A6P4	4.009601	A10P4	4.010521
P3	4.007434	A3	3.998172	A2P6	4.002766	A6P6	4.009068	A10P6	4.017448
P4	4.007593	A4	3.99817	A2P8	4.004845	A6P8	4.004356	A10P8	4.000412
P5	4.006012	A5	3.99817	A2P10	4.005104	A6P10	4.005673	A10P10	4.003998
P6	4.009703	A6	4.001715	A2P12	4.004352	A6P12	4.004874	A10P12	4.0055
P7	4.001785	A7	3.998175	A4P2	4.006152	A8P2	4.0077	A12P2	4.006407
P8	4.000934	A8	4.001844	A4P4	4.004603	A8P4	4.004102	A12P4	4.008879
P9	4.000049	A9	4.000972	A4P6	4.005796	A8P6	3.998178	A12P6	4.003763
P10	4.001988	A10	3.998172	A4P8	4.001145	A8P8	4.004602	A12P8	4.010997
P11	4.003432	A11	4.002367	A4P10	4.010525	A8P10	4.004874	A12P10	4.007935
P12	3.998182	A12	4.000505	A4P12	4.002458	A8P12	4.001679	A12P12	3.998176
P13	4.006033	A13	3.998178						
P14	4.016041	A14	4.002625						

#### Ca-O

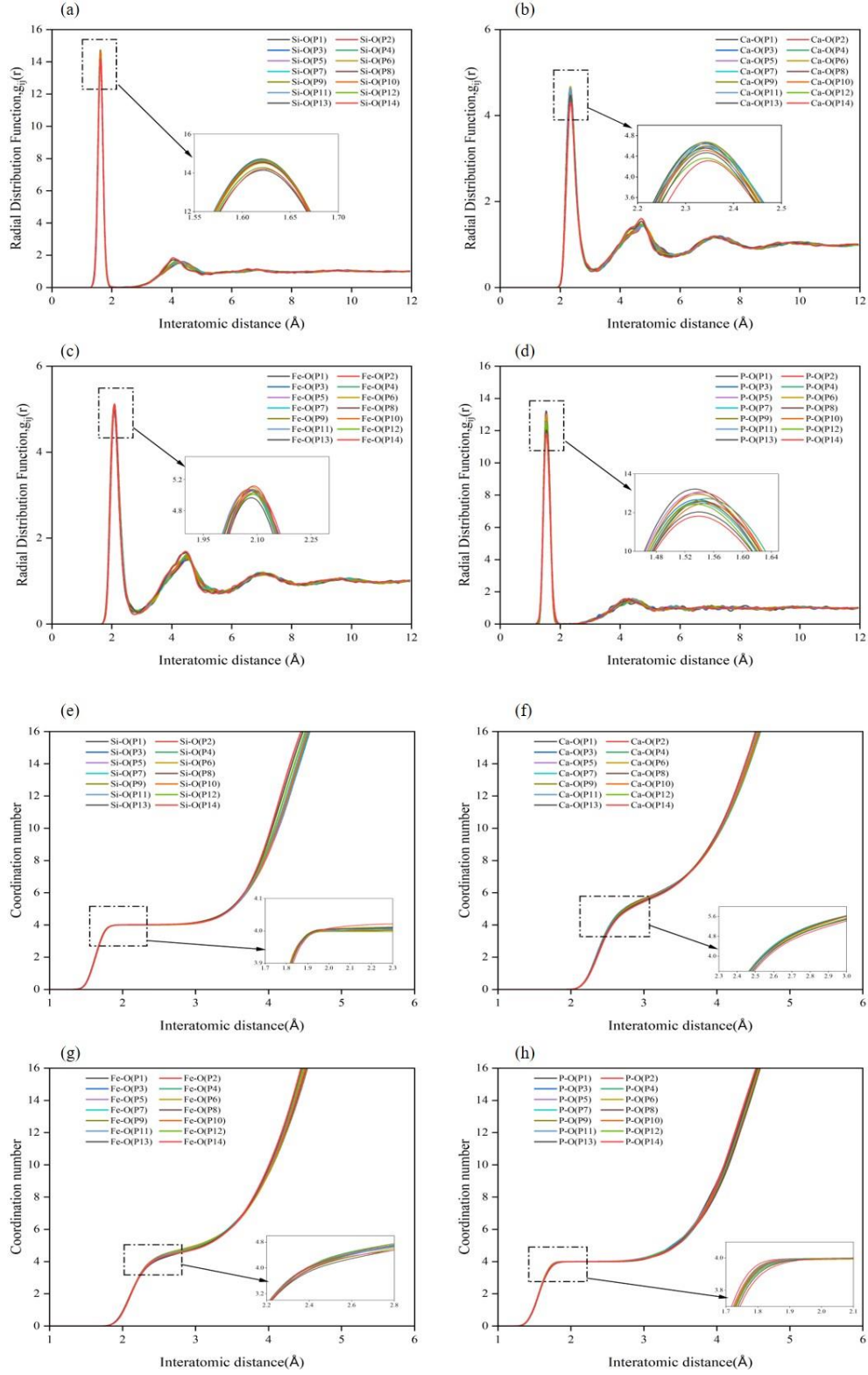
P1	5.744784	A1	5.595522	A2P2	5.773589	A6P2	5.729697	A10P2	5.75438
P2	5.752946	A2	5.545163	A2P4	5.726512	A6P4	5.708809	A10P4	5.708831
P3	5.736012	A3	5.544894	A2P6	5.72684	A6P6	5.703893	A10P6	5.694178
P4	5.722477	A4	5.54196	A2P8	5.708811	A6P8	5.654421	A10P8	5.696346
P5	5.724736	A5	5.534622	A2P10	5.657105	A6P10	5.67686	A10P10	5.688987
P6	5.720999	A6	5.555096	A2P12	5.674269	A6P12	5.683833	A10P12	5.696882
P7	5.746313	A7	5.512343	A4P2	5.766749	A8P2	5.774306	A12P2	5.749801
P8	5.741697	A8	5.558229	A4P4	5.714269	A8P4	5.750076	A12P4	5.736179
P9	5.725852	A9	5.50412	A4P6	5.694343	A8P6	5.706273	A12P6	5.710655
P10	5.733124	A10	5.507762	A4P8	5.724212	A8P8	5.710183	A12P8	5.721638
P11	5.662905	A11	5.500191	A4P10	5.686432	A8P10	5.718602	A12P10	5.657431
P12	5.629677	A12	5.535887	A4P12	5.686184	A8P12	5.691885	A12P12	5.67533
P13	5.609797	A13	5.529829						
P14	5.555363	A14	5.542325						

#### Fe-O

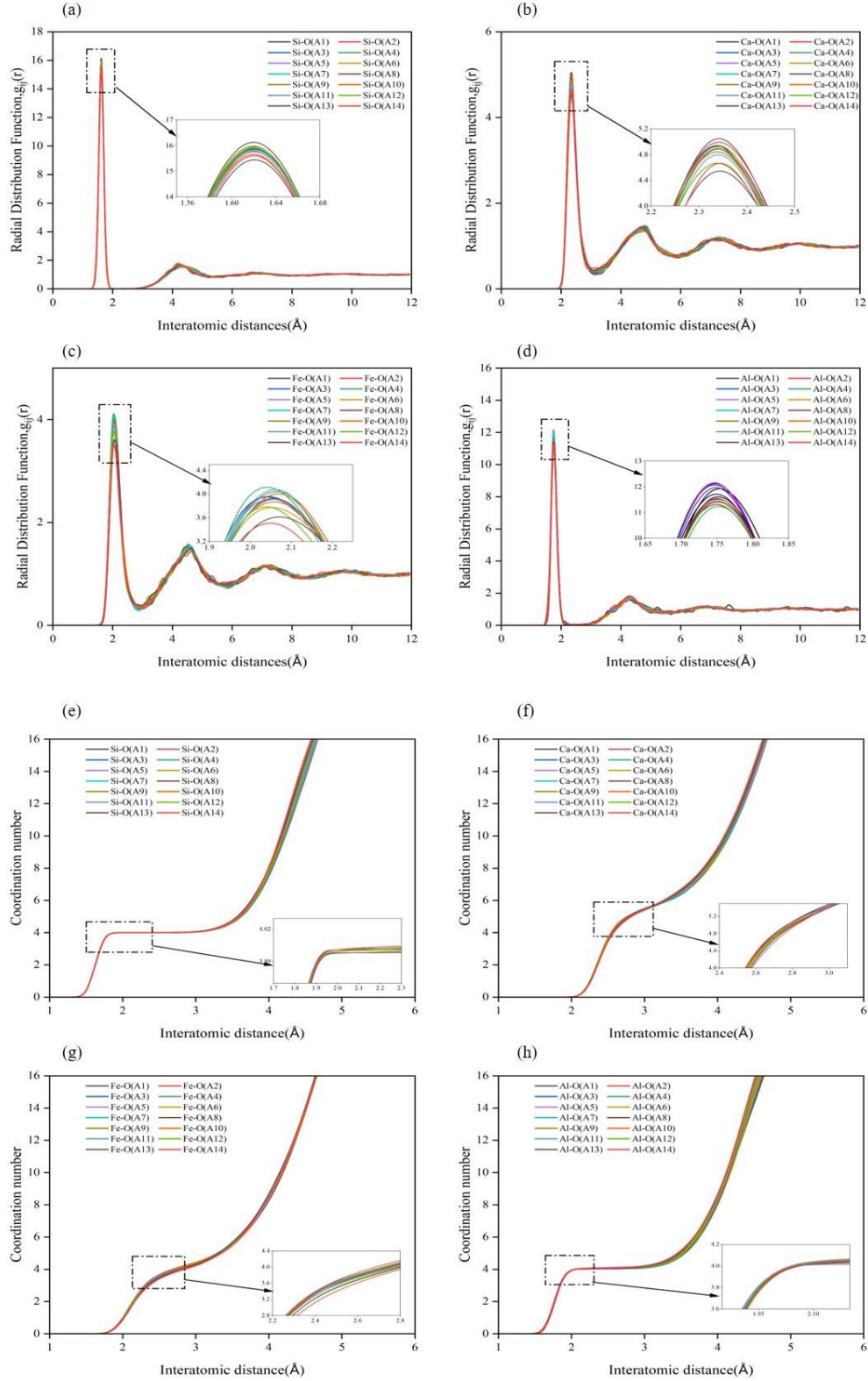
P1	5.276981	A1	5.197182	A2P2	5.277189	A6P2	5.249172	A10P2	5.232672
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P2	5.290074	A2	5.317126	A2P4	5.231924	A6P4	5.222669	A10P4	5.176774
P3	5.243304	A3	5.284381	A2P6	5.199089	A6P6	5.214325	A10P6	5.150592
P4	5.231989	A4	5.23165	A2P8	5.179709	A6P8	5.176774	A10P8	5.228285
P5	5.218822	A5	5.221628	A2P10	5.222067	A6P10	5.256131	A10P10	5.202093
P6	5.279107	A6	5.285544	A2P12	5.255179	A6P12	5.166955	A10P12	5.20098
P7	5.237808	A7	5.211527	A4P2	5.22921	A8P2	5.258319	A12P2	5.140809
P8	5.212746	A8	5.202816	A4P4	5.270116	A8P4	5.206069	A12P4	5.217253
P9	5.209494	A9	5.26157	A4P6	5.228157	A8P6	5.212751	A12P6	5.110276
P10	5.161434	A10	5.214526	A4P8	5.204612	A8P8	5.201514	A12P8	5.163856
P11	5.224235	A11	5.28847	A4P10	5.221968	A8P10	5.192964	A12P10	5.19256
P12	5.219294	A12	5.307578	A4P12	5.219102	A8P12	5.131207	A12P12	5.10308
P13	5.143085	A13	5.3538						
P14	5.073995	A14	5.185146						

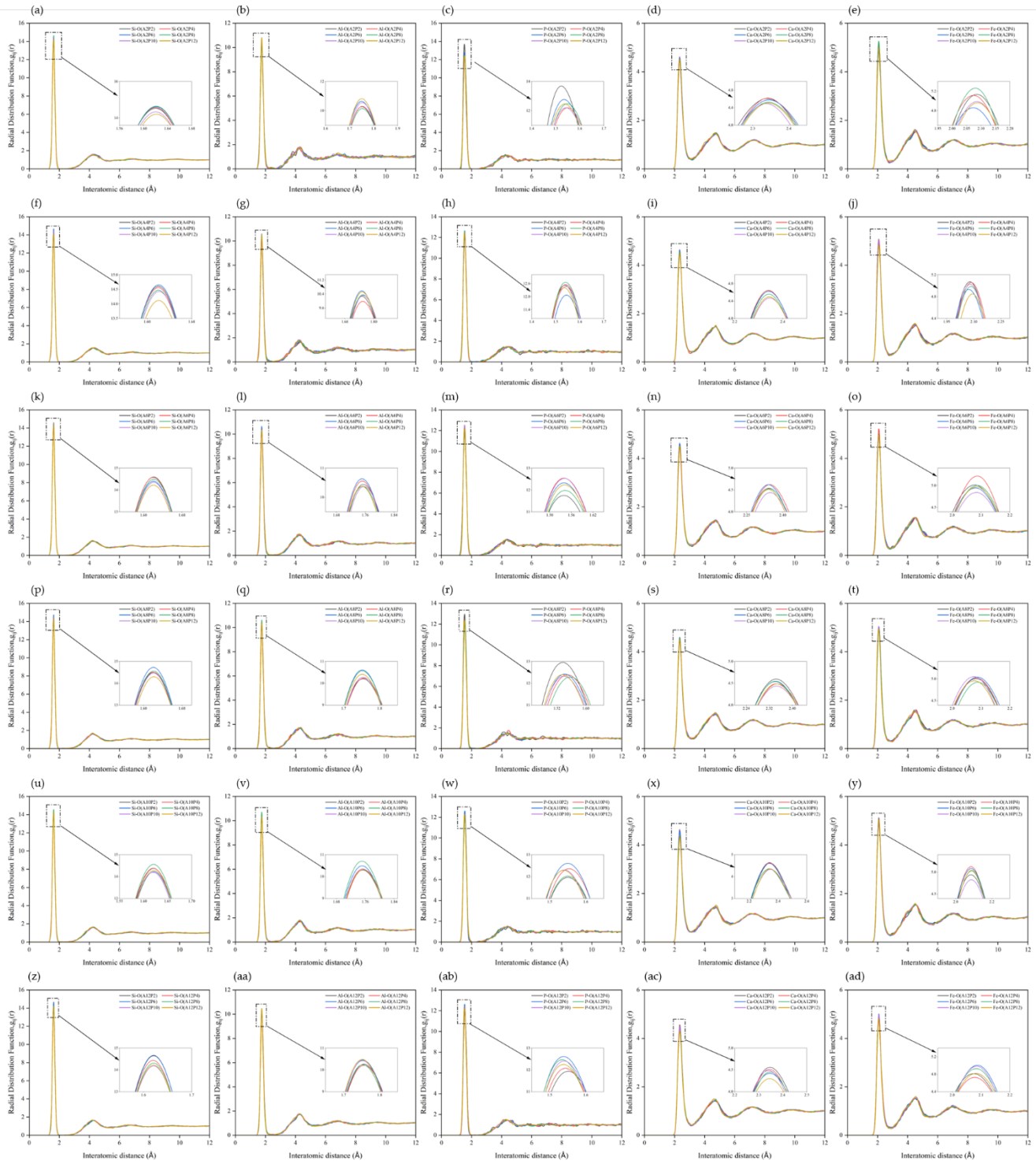
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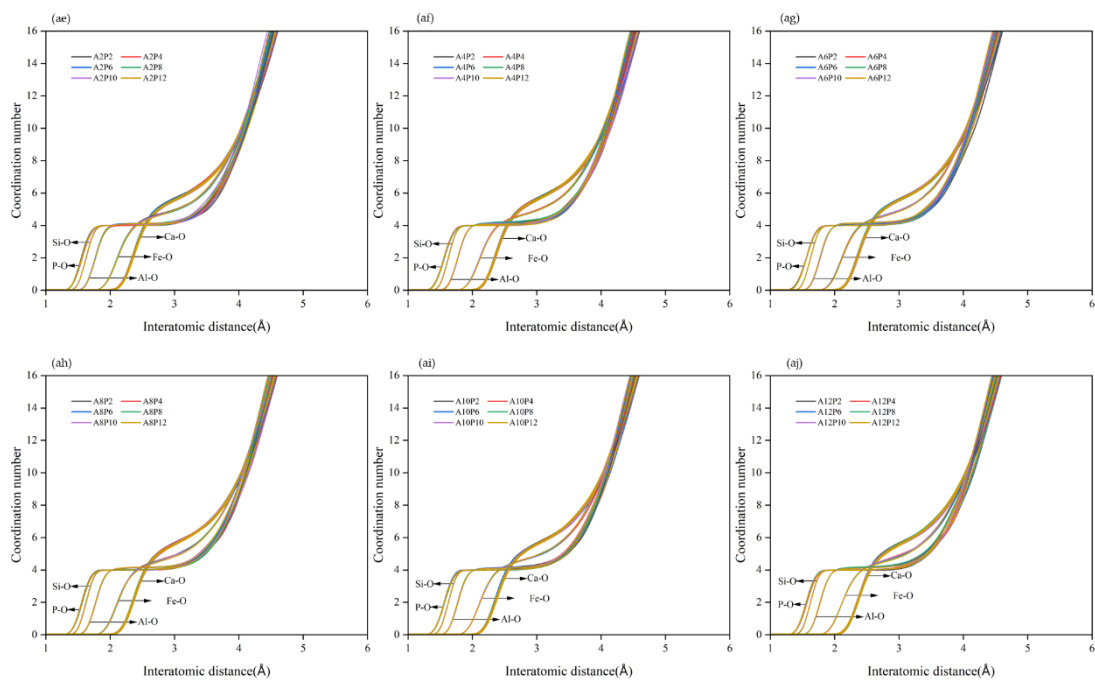
**Figure S1.** Radial distribution function and coordination numbers of the major atomic pairs in the P models: (a), (b), (c), (d): RDF of P models; (e), (f), (g), (h): CN of P models.



**Figure S2.** Radial distribution function and coordination numbers of the major atomic pairs in the A models: (a), (b), (c), (d): RDF of A models; (e), (f), (g), (h): CN of A models.







**Figure S3.** Radial distribution function and coordination numbers of the main atomic pairs in the AP models:(a-ad) radial distribution function of the main atomic pairs in the AP models; (ae-aj) coordination numbers of the main atomic pairs in the AP models.