

Supplementary Information (SI)

Predicting the pair correlation functions of silicate and borosilicate glasses using machine learning

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1) Composition corresponding to the training data

The table provides the composition corresponding to each of the 184 datapoints used for training the model. It includes base compound(glass), dopant, concentration of dopant(mol%) and the pair of atoms between which the PCF is considered.

S. No.	Base Compound	Dopant	Concentration of dopants (mol%)	Pair of Atoms
1	Silicate	BaO	70	Si-Ba
2	Sodium Borosilicate	ZnO	9.8	Na-Zn
3	Sodium Borosilicate	TiO ₂	4.77	Si-Si
4	Sodium Borosilicate	ZnO	9.8	O-O
5	Sodium Borosilicate	TiO ₂	19.97	Ti-Na
6	Sodium Borosilicate	TiO ₂	9.1	Si-Na
7	Sodium Borosilicate	TiO ₂	19.97	B-Ti
8	Sodium Borosilicate	TiO ₂	1.95	Na-O
9	Sodium Borosilicate	TiO ₂	13.06	Ti-O
10	Sodium Silicate	ZnO	10	Zn-Zn
11	Sodium Borosilicate	TiO ₂	4.77	B-Na
12	Silicate	BaO	50	Si-Si
13	Sodium Borosilicate	BaO	1.95	O-O
14	Silicate	BaO	70	Ba-Ba
15	Sodium Borosilicate	None	0	Si-Si
16	Sodium Silicate	ZnO	10	B-B
17	Sodium Borosilicate	BaO	9.1	B-O
18	Sodium Borosilicate	TiO ₂	16.69	B-Na
19	Silicate	BaO	30	O-O
20	Sodium Borosilicate	TiO ₂	4.77	Si-O
21	Sodium Borosilicate	TiO ₂	1.95	Si-Si
22	Sodium Borosilicate	TiO ₂	4.77	B-Ti
23	Silicate	BaO	30	Si-O
24	Sodium Borosilicate	BaO	1.95	B-Ba
25	Sodium Borosilicate	TiO ₂	16.69	Si-B

26	Sodium Borosilicate	TiO ₂	19.97	Ti-O
27	Sodium Borosilicate	ZnO	12.6	Na-Na
28	Silicate	BaO	30	Ba-Ba
29	Sodium Borosilicate	TiO ₂	9.1	Ti-Ti
30	Sodium Silicate	ZnO	10	Na-Na
31	Sodium Borosilicate	TiO ₂	9.1	Ti-O
32	Silicate	BaO	70	O-O
33	Sodium Borosilicate	BaO	1.95	Ba-O
34	Sodium Borosilicate	BaO	13.06	Si-Si
35	Silicate	BaO	10	O-O
36	Sodium Borosilicate	BaO	9.1	Si-B
37	Sodium Borosilicate	ZnO	6.1	Na-Zn
38	Sodium Borosilicate	TiO ₂	19.97	Si-B
39	Sodium Borosilicate	TiO ₂	13.06	Si-O
40	Sodium Borosilicate	BaO	13.06	Si-Ba
41	Sodium Borosilicate	TiO ₂	16.69	Na-O
42	Sodium Borosilicate	ZnO	12.6	Si-Si
43	Sodium Borosilicate	TiO ₂	9.1	B-Ti
44	Sodium Borosilicate	BaO	4.77	Si-B
45	Sodium Borosilicate	TiO ₂	19.97	Ti-O
46	Sodium Borosilicate	TiO ₂	1.95	Ti-Ti
47	Sodium Borosilicate	TiO ₂	16.69	B-Ti
48	Sodium Borosilicate	TiO ₂	4.77	Ti-O
49	Sodium Borosilicate	BaO	9.1	O-O
50	Sodium Silicate	ZnO	10	B-Na
51	Sodium Borosilicate	None	0	Si-Na
52	Sodium Silicate	ZnO	10	Zn-O
53	Sodium Borosilicate	BaO	1.95	Si-O
54	Sodium Borosilicate	BaO	9.1	Si-O
55	Sodium Borosilicate	TiO ₂	13.06	B-Ti
56	Sodium Borosilicate	BaO	9.1	B-B
57	Sodium Borosilicate	TiO ₂	9.1	B-O
58	Sodium Borosilicate	TiO ₂	4.77	Si-B
59	Sodium Borosilicate	TiO ₂	16.69	Ti-O
60	Silicate	ZnO	20	O-O
61	Sodium Borosilicate	TiO ₂	16.69	Na-O
62	Sodium Borosilicate	TiO ₂	19.97	Si-Ti
63	Sodium Borosilicate	ZnO	9.8	Zn-O
64	Sodium Borosilicate	TiO ₂	1.95	Si-O
65	Sodium Borosilicate	TiO ₂	1.95	B-O
66	Silicate	BaO	10	Si-Si
67	Sodium Borosilicate	ZnO	9.8	Si-O
68	Sodium Borosilicate	BaO	4.77	Ba-Ba
69	Sodium Borosilicate	BaO	9.1	Na-O
70	Silicate	ZnO	20	Zn-Zn
71	Sodium Silicate	None	0	Si-Si
72	Sodium Borosilicate	BaO	4.77	Si-Si

73	Sodium Borosilicate	BaO	13.06	B-O
74	Sodium Silicate	None	0	B-Zn
75	Sodium Borosilicate	None	0	Si-O
76	Silicate	BaO	50	Si-O
77	Sodium Borosilicate	BaO	13.06	O-O
78	Sodium Borosilicate	TiO ₂	4.77	Ti-Ti
79	Sodium Borosilicate	None	0	Zn-Zn
80	Sodium Borosilicate	ZnO	6.1	Zn-Zn
81	Sodium Borosilicate	TiO ₂	16.69	Si-O
82	Silicate	BaO	10	Si-O
83	Sodium Borosilicate	TiO ₂	1.95	Si-Na
84	Sodium Borosilicate	BaO	1.95	Si-Si
85	Sodium Silicate	ZnO	10	O-O
86	Sodium Borosilicate	BaO	9.1	Ba-Ba
87	Sodium Borosilicate	TiO ₂	1.95	Na-O
88	Sodium Silicate	ZnO	10	Na-O
89	Sodium Borosilicate	ZnO	6.1	Si-Na
90	Sodium Borosilicate	TiO ₂	9.1	Si-Si
91	Sodium Borosilicate	None	0	Si-O
92	Silicate	BaO	10	Ba-Ba
93	Sodium Borosilicate	BaO	1.95	B-B
94	Sodium Borosilicate	TiO ₂	9.1	B-B
95	Sodium Borosilicate	BaO	1.95	Si-B
96	Sodium Borosilicate	TiO ₂	4.77	Si-Na
97	Sodium Borosilicate	BaO	13.06	Na-O
98	Sodium Silicate	ZnO	10	Si-Na
99	Sodium Borosilicate	ZnO	6.1	O-O
100	Sodium Borosilicate	TiO ₂	4.77	Si-Ti
101	Silicate	BaO	70	Si-Si
102	Sodium Borosilicate	ZnO	9.8	Na-Na
103	Sodium Borosilicate	BaO	13.06	B-B
104	Sodium Borosilicate	TiO ₂	9.1	Ti-O
105	Sodium Borosilicate	None	0	Na-Na
106	Sodium Borosilicate	BaO	13.06	Si-B
107	Sodium Borosilicate	TiO ₂	19.97	Ti-Ti
108	Sodium Borosilicate	ZnO	12.6	Na-O
109	Sodium Borosilicate	BaO	13.06	Si-O
110	Sodium Borosilicate	TiO ₂	4.77	Ti-Na
111	Silicate	BaO	30	Si-Ba
112	Sodium Borosilicate	TiO ₂	19.97	Na-O
113	Sodium Borosilicate	ZnO	6.1	Na-O
114	Sodium Borosilicate	ZnO	6.1	Si-O
115	Silicate	ZnO	20	B-Na
116	Sodium Borosilicate	BaO	4.77	Si-Ba
117	Sodium Silicate	None	0	O-O
118	Sodium Borosilicate	TiO ₂	1.95	Si-Ti
119	Sodium Borosilicate	BaO	9.1	Si-Si

120	Silicate	BaO	70	Si-O
121	Sodium Borosilicate	TiO ₂	1.95	Si-B
122	Sodium Borosilicate	TiO ₂	19.97	Na-O
123	Sodium Borosilicate	TiO ₂	13.06	Si-Ti
124	Sodium Borosilicate	ZnO	6.1	Na-O
125	Sodium Borosilicate	ZnO	9.8	Na-O
126	Sodium Borosilicate	TiO ₂	13.06	Na-O
127	Sodium Borosilicate	BaO	1.95	B-O
128	Sodium Borosilicate	BaO	4.77	Ba-O
129	Sodium Borosilicate	BaO	13.06	B-Ba
130	Sodium Borosilicate	ZnO	9.8	B-B
131	Sodium Borosilicate	TiO ₂	13.06	Na-O
132	Silicate	BaO	30	Ba-O
133	Sodium Borosilicate	None	0	O-O
134	Sodium Borosilicate	TiO ₂	16.69	Si-Si
135	Sodium Borosilicate	ZnO	6.1	B-O
136	Sodium Borosilicate	TiO ₂	1.95	Ti-O
137	Sodium Borosilicate	ZnO	12.6	B-Zn
138	Sodium Silicate	None	0	B-Na
139	Sodium Borosilicate	BaO	13.06	Ba-Ba
140	Silicate	BaO	50	Si-Ba
141	Sodium Borosilicate	TiO ₂	13.06	Ti-Na
142	Sodium Borosilicate	BaO	9.1	Si-Ba
143	Sodium Borosilicate	ZnO	9.8	Si-Na
144	Sodium Borosilicate	ZnO	12.6	B-O
145	Sodium Borosilicate	ZnO	12.6	Si-Si
146	Sodium Borosilicate	None	0	Na-Zn
147	Sodium Borosilicate	ZnO	12.6	Zn-Si
148	Sodium Borosilicate	ZnO	12.6	O-O
149	Sodium Borosilicate	BaO	9.1	B-Ba
150	Sodium Borosilicate	BaO	1.95	Si-Ba
151	Sodium Borosilicate	TiO ₂	9.1	Na-O
152	Sodium Borosilicate	BaO	4.77	Na-O
153	Sodium Borosilicate	BaO	4.77	B-Ba
154	Sodium Borosilicate	ZnO	6.1	Zn-O
155	Sodium Borosilicate	ZnO	9.8	Zn-Zn
156	Sodium Borosilicate	ZnO	6.1	Si-Si
157	Sodium Borosilicate	ZnO	6.1	Na-Na
158	Sodium Borosilicate	TiO ₂	4.77	Na-O
159	Silicate	BaO	30	Si-Si
160	Sodium Borosilicate	TiO ₂	19.97	Si-O
161	Sodium Borosilicate	ZnO	9.8	Zn-Si
162	Sodium Borosilicate	BaO	4.77	Si-O
163	Silicate	BaO	10	Si-Ba
164	Sodium Borosilicate	TiO ₂	13.06	B-B
165	Sodium Borosilicate	TiO ₂	9.1	Na-O
166	Sodium Borosilicate	TiO ₂	19.97	B-B

167	Sodium Borosilicate	TiO ₂	19.97	B-O
168	Sodium Borosilicate	TiO ₂	4.77	B-O
169	Sodium Borosilicate	TiO ₂	1.95	B-Na
170	Sodium Borosilicate	TiO ₂	4.77	Na-O
171	Sodium Borosilicate	ZnO	9.8	B-O
172	Sodium Borosilicate	TiO ₂	1.95	B-Ti
173	Sodium Borosilicate	None	0	Zn-Si
174	Sodium Borosilicate	ZnO	12.6	B-Na
175	Sodium Borosilicate	TiO ₂	19.97	B-Na
176	Sodium Borosilicate	ZnO	12.6	Na-Zn
177	Sodium Borosilicate	BaO	1.95	Na-O
178	Sodium Borosilicate	ZnO	9.8	Si-Si
179	Sodium Borosilicate	TiO ₂	13.06	Si-Si
180	Sodium Borosilicate	TiO ₂	9.1	Ti-Na
181	Sodium Borosilicate	BaO	9.1	Ba-O
182	Sodium Borosilicate	TiO ₂	1.95	Ti-O
183	Sodium Borosilicate	ZnO	12.6	Si-O
184	Sodium Borosilicate	TiO ₂	16.69	B-O

2) Composition corresponding to the test data

The table provides the composition corresponding to each of the test dataset (47 points) used for testing the performance of the model. It includes base compound(glass), dopant, concentration of dopant(mol%) and the pair of atoms between which the PCF is considered.

S. No.	Base Compound	Dopant	Concentration of dopants (mol%)	Pair of Atoms
1	Sodium Silicate	None	0	Zn-Si
2	Silicate	BaO	50	Ba-Ba
3	Sodium Borosilicate	BaO	4.77	B-O
4	Sodium Silicate	None	0	Si-Na
5	Sodium Borosilicate	BaO	13.06	Ba-O
6	Silicate	ZnO	20	B-O
7	Sodium Borosilicate	BaO	4.77	O-O
8	Sodium Borosilicate	ZnO	6.1	B-B
9	Sodium Borosilicate	TiO ₂	9.1	Si-O
10	Sodium Borosilicate	TiO ₂	16.69	Si-Na
11	Sodium Borosilicate	ZnO	6.1	Zn-Si
12	Silicate	BaO	70	Ba-O
13	Sodium Borosilicate	TiO ₂	16.69	Ti-O
14	Sodium Borosilicate	ZnO	9.8	Si-O
15	Sodium Borosilicate	ZnO	12.6	Si-Na
16	Sodium Borosilicate	TiO ₂	13.06	Ti-O
17	Sodium Borosilicate	TiO ₂	1.95	B-B
18	Silicate	BaO	50	O-O
19	Sodium Silicate	ZnO	10	B-Zn
20	Sodium Silicate	ZnO	10	Si-Si
21	Sodium Borosilicate	TiO ₂	16.69	Ti-Na
22	Sodium Borosilicate	ZnO	12.6	Zn-O
23	Sodium Borosilicate	ZnO	9.8	Na-O
24	Sodium Borosilicate	ZnO	6.1	Si-O
25	Sodium Borosilicate	TiO ₂	13.06	Si-Na
26	Silicate	BaO	50	Ba-O
27	Sodium Borosilicate	TiO ₂	4.77	B-B
28	Sodium Borosilicate	TiO ₂	13.06	B-O
29	Sodium Borosilicate	TiO ₂	1.95	Ti-Na
30	Sodium Borosilicate	TiO ₂	16.69	Si-Ti
31	Sodium Borosilicate	ZnO	12.6	B-B
32	Sodium Borosilicate	BaO	1.95	Ba-Ba
33	Sodium Borosilicate	TiO ₂	9.1	B-Na
34	Sodium Borosilicate	BaO	4.77	B-B
35	Silicate	BaO	10	Ba-O
36	Sodium Borosilicate	TiO ₂	19.97	Si-Na
37	Silicate	ZnO	20	Zn-O
38	Sodium Borosilicate	TiO ₂	13.06	B-Na
39	Sodium Borosilicate	TiO ₂	9.1	Si-Ti

40	Sodium Borosilicate	TiO ₂	16.69	Ti-Ti
41	Sodium Borosilicate	TiO ₂	4.77	Ti-O
42	Silicate	ZnO	20	Na-Na
43	Sodium Borosilicate	TiO ₂	13.06	Ti-Ti
44	Sodium Borosilicate	TiO ₂	19.97	Si-Si
45	Sodium Borosilicate	TiO ₂	13.06	Si-B
46	Sodium Borosilicate	TiO ₂	9.1	Si-B
47	Sodium Borosilicate	TiO ₂	16.69	B-B

3) Composition table for each RDF in Figure 9 of the main text

Figure 9 in the main text displays nine Pair Correlation Functions (PCF) depicting both actual and predicted curves. The composition details of these functions are provided below.

S. No.	Base Compound	Dopant	Concentration of dopants (mol%)	Pair of Atoms
1	Sodium Silicate	None	0	Zn-Si
2	Silicate	BaO	50	Ba-Ba
3	Sodium Borosilicate	BaO	4.77	B-O
4	Sodium Silicate	None	0	Si-Na
5	Sodium Borosilicate	BaO	13.06	Ba-O
6	Silicate	ZnO	20	B-O
7	Sodium Borosilicate	BaO	4.77	O-O
8	Sodium Borosilicate	ZnO	6.1	B-B
9	Sodium Borosilicate	TiO ₂	9.1	Si-O