Automated Pair Distribution Function Analysis for Assessing Reaction Progress

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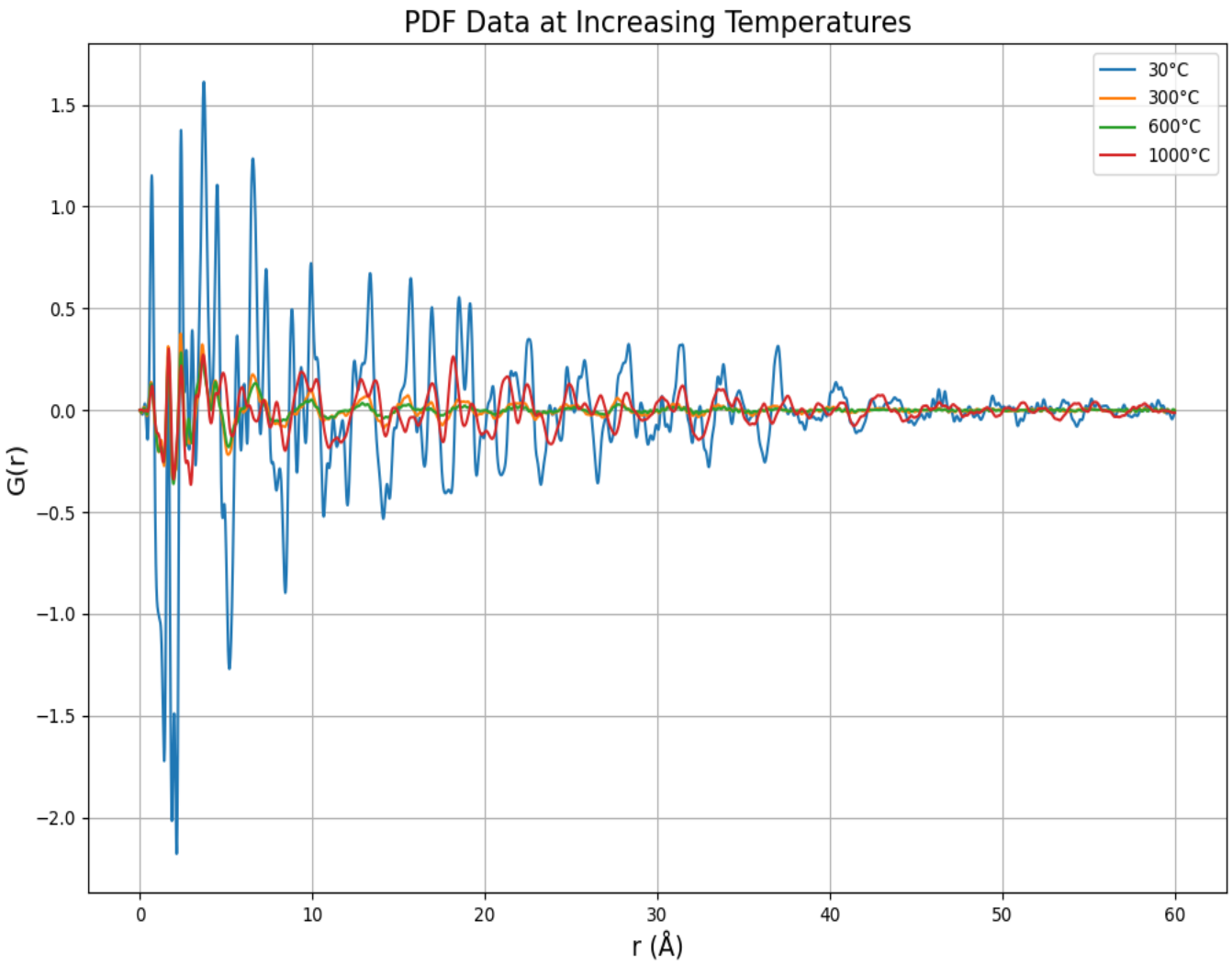
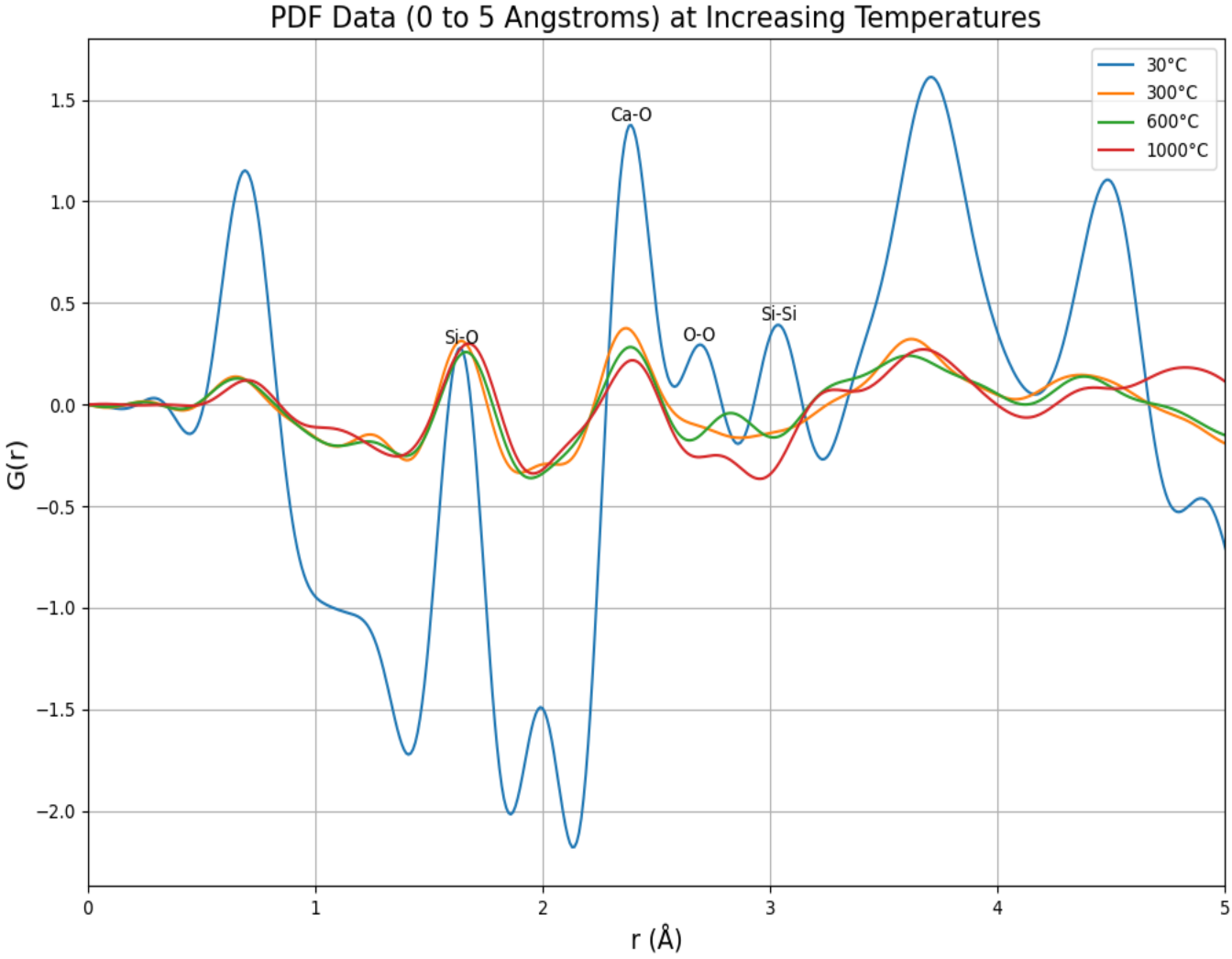
Section 1: PDF Curve Plotting

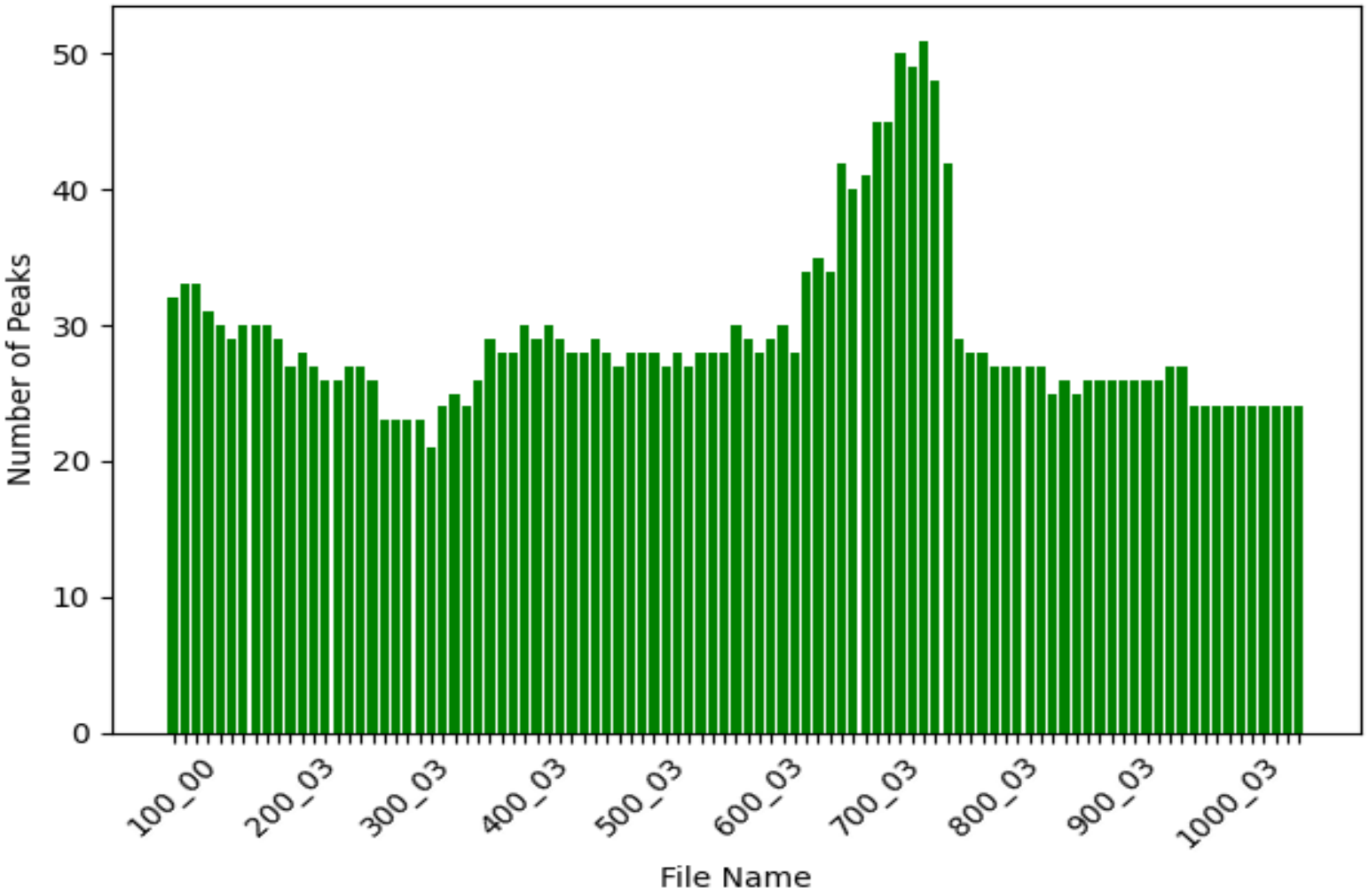
This section visualizes the PDF data




PDF Data (0 to 5 Angstroms) at Increasing Temperatures
30°C
300°C
600°C
1000°C
Ca-O
Si-O
O-O
Si-Si
G(r)
r (Å)
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
1
2
3
4
5

Section 2: Visualizing Total Number of Peaks Over Time

This section visualizes phase changes by counting the total number of peaks in PDF files across temperatures



Section 3: Quantifying Peak Positions

The results of quanitfying peak postions are in text file called tracked_peak_matrix.txt in the data folder!

Section 4: Peak Integration

This table lists relative differences between reference peak integrals (denoted 0) at a given temperature and peak integrals calculated at higher temperatures. These values are indicative of changes that occur to atomic coordination numbers as the structure of C-S-H changes

	Peak 1	Peak 2	Peak 3	Peak 4
100°C	0.0	0.0	0.0	0.0
200°C	0.0	0.4	1.8	1.6
300°C	0.0	3.7	0.4	3.2
400°C	0.0	0.3	2.1	3.9
500°C	0.0	0.5	2.0	4.4
600°C	0.0	1.8	2.2	5.4
700°C	0.0	2.8	2.0	6.8
800°C	0.0	1.7	2.7	10.2
900°C	0.0	2.0	3.4	10.4