# Automated Pair Distribution Function Analysis for Assessing Reaction Progress

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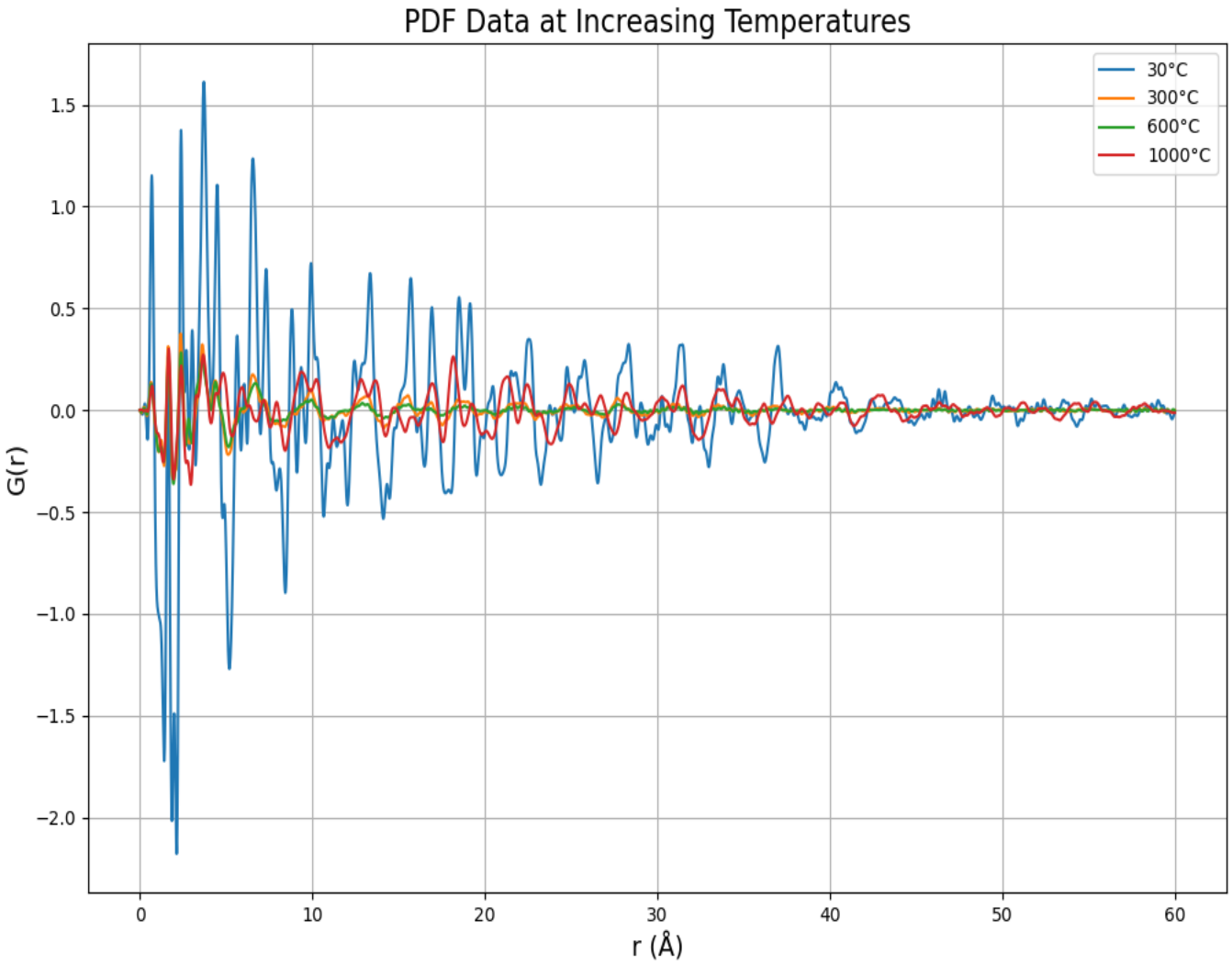
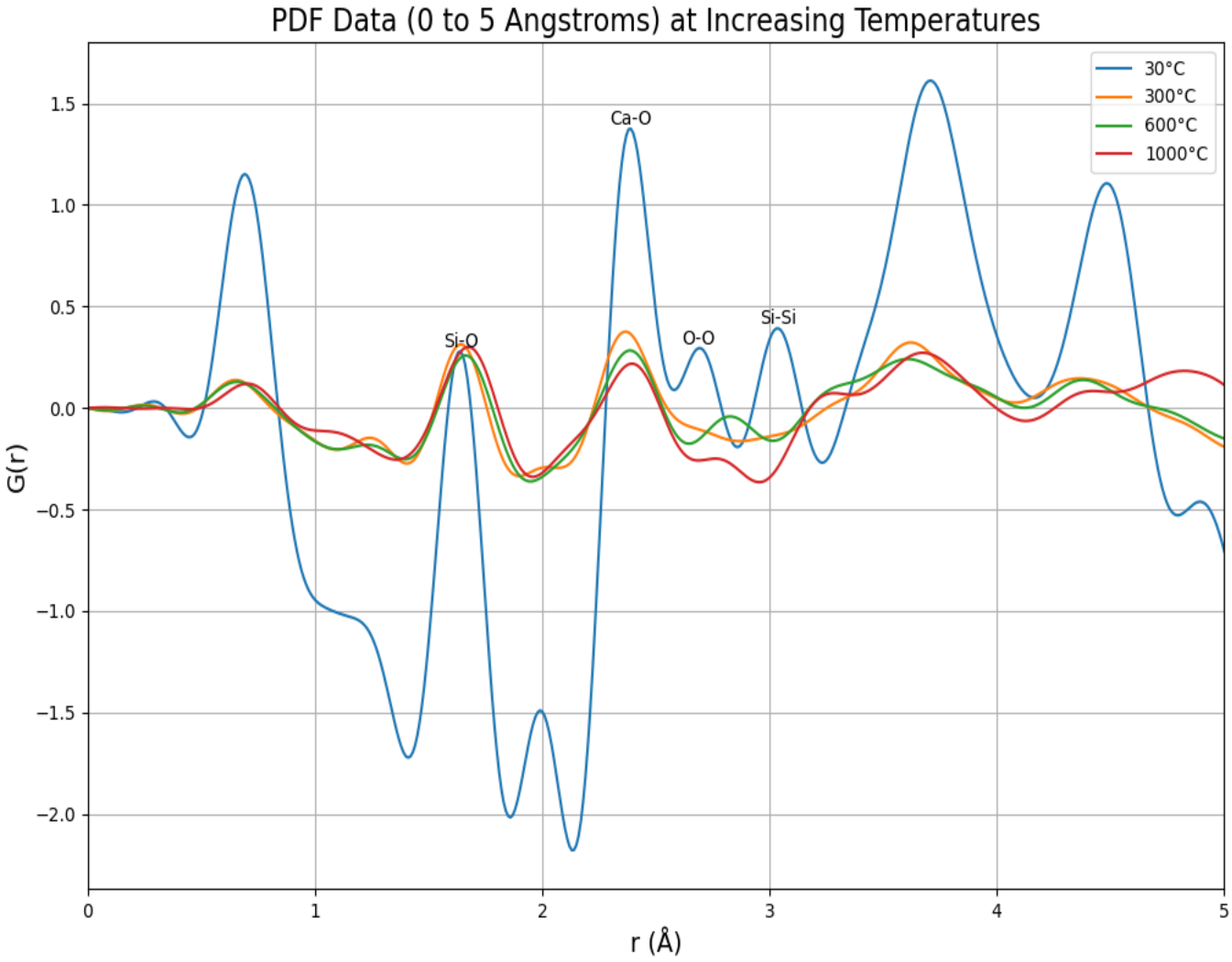
# Section 1: PDF Curve Plotting

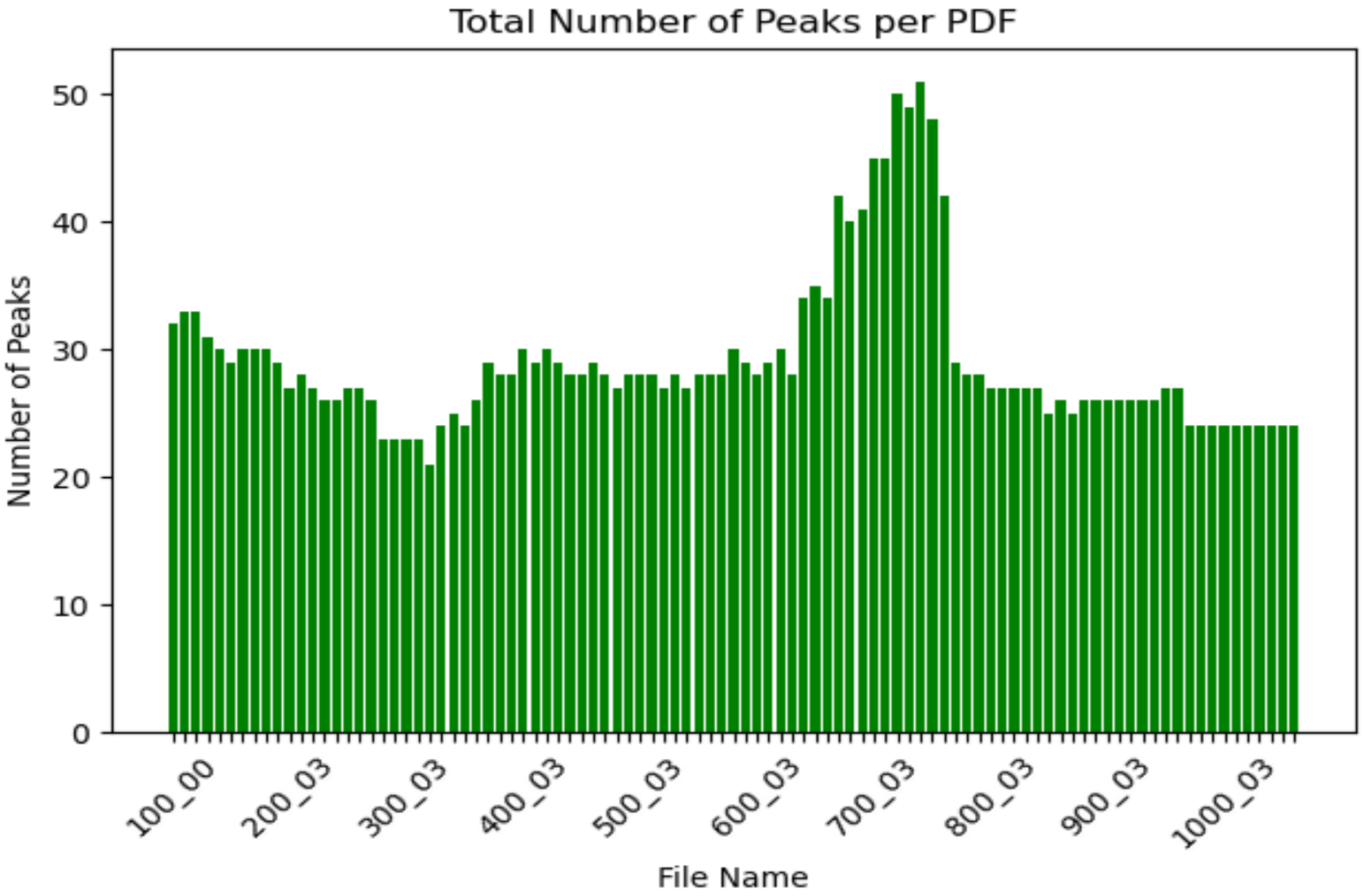
This section visualizes the PDF data.




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.

Relative Changes to Atomic Coordination Numbers with Temperature

| | 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 |