Supplementary Document

Supplementary document for

Fracture Toughness of Sodium Aluminosilicate Hydrate (NASH) Gels: Insights from Molecular Dynamics Simulations

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A. Partial PDF of Na-X (X=Al, Si, Na, O, Ow, H):

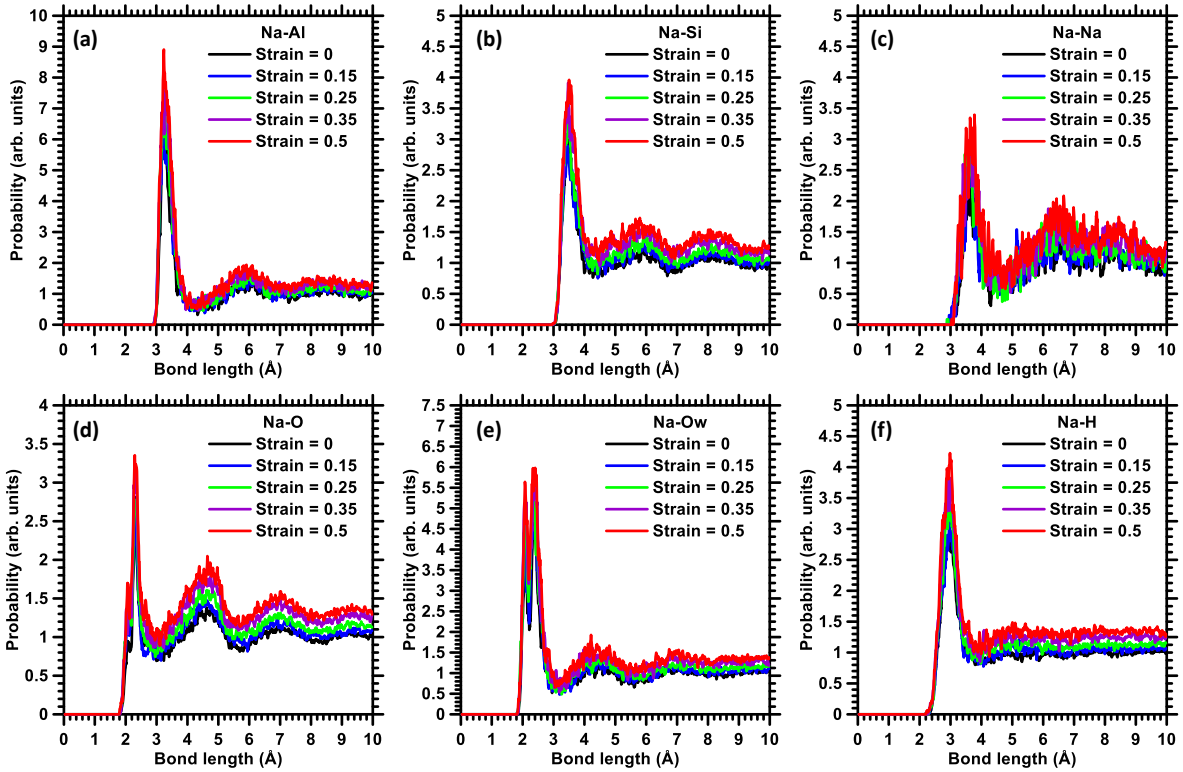

Figure 1. PDFs for: (a) Na-Al, (b) Na-Si, (c) Na-Na, (d) Na-O, (e) Na-Ow, and (f) Na-H pairs with varying strain.

B. Cutoff distance

Table 1 presents the cutoff distance used to assess the nature of pair atoms during fracture. The cutoff distance is chosen as the first minimum after the first peak of the partial PDF.

Table 1: Cut-off distances used in the analysis to assess the nature of pair atoms during fracture

Pair atoms	Cut-off (Å)	Pair atoms	Cut-off (Å)
Al-O	2.2	Na-Al	4.0
Si-O	2.0	Na-Si	4.0
Na-O	3.0	Al-Al	3.4
Na-Na	4.0	Al-Si	4.0
O-H	1.35	Na-H	3.0