

*Supporting Information for*

**Molecular Insights into the Temperature and Pressure Dependence of Mechanical  
Behavior and Dynamics of Na-Montmorillonite Clay**

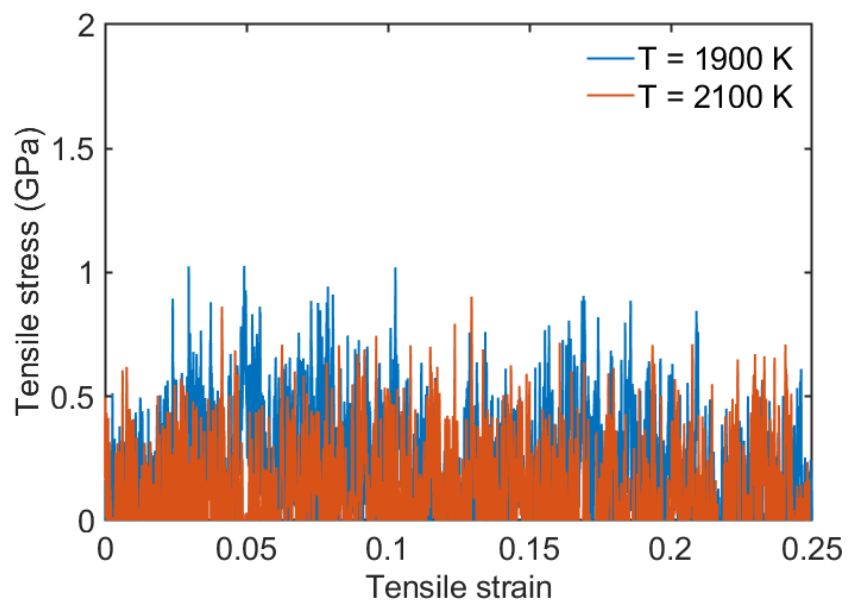
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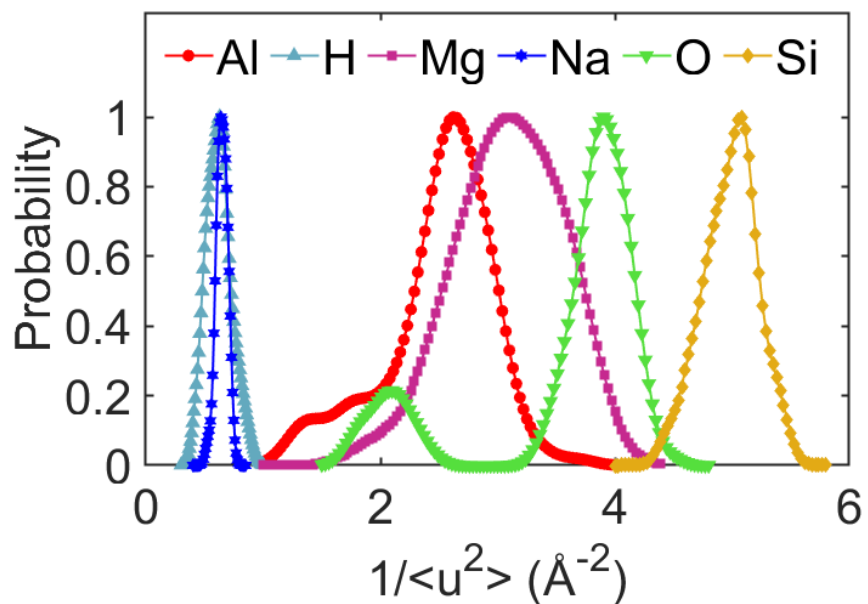
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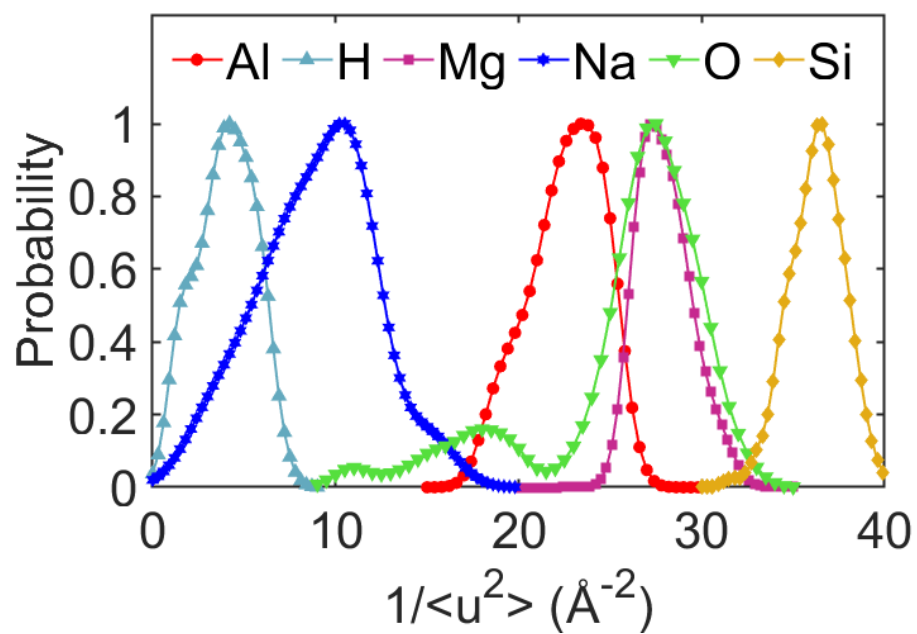
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**Figure S1.** Tensile test for temperatures out of selected range when the pressure is 1000 atm.



**Figure S2.** Probability distribution of local molecular stiffness  $1/\langle u^2 \rangle$  of the Na-MMT system for different atom types undergoing zero pressure and 1700 K temperature.



**Figure S3.** Probability distribution of local molecular stiffness  $1/\langle u^2 \rangle$  of the Na-MMT system for different atom types undergoing 1000 atm pressure and 300 K temperature.