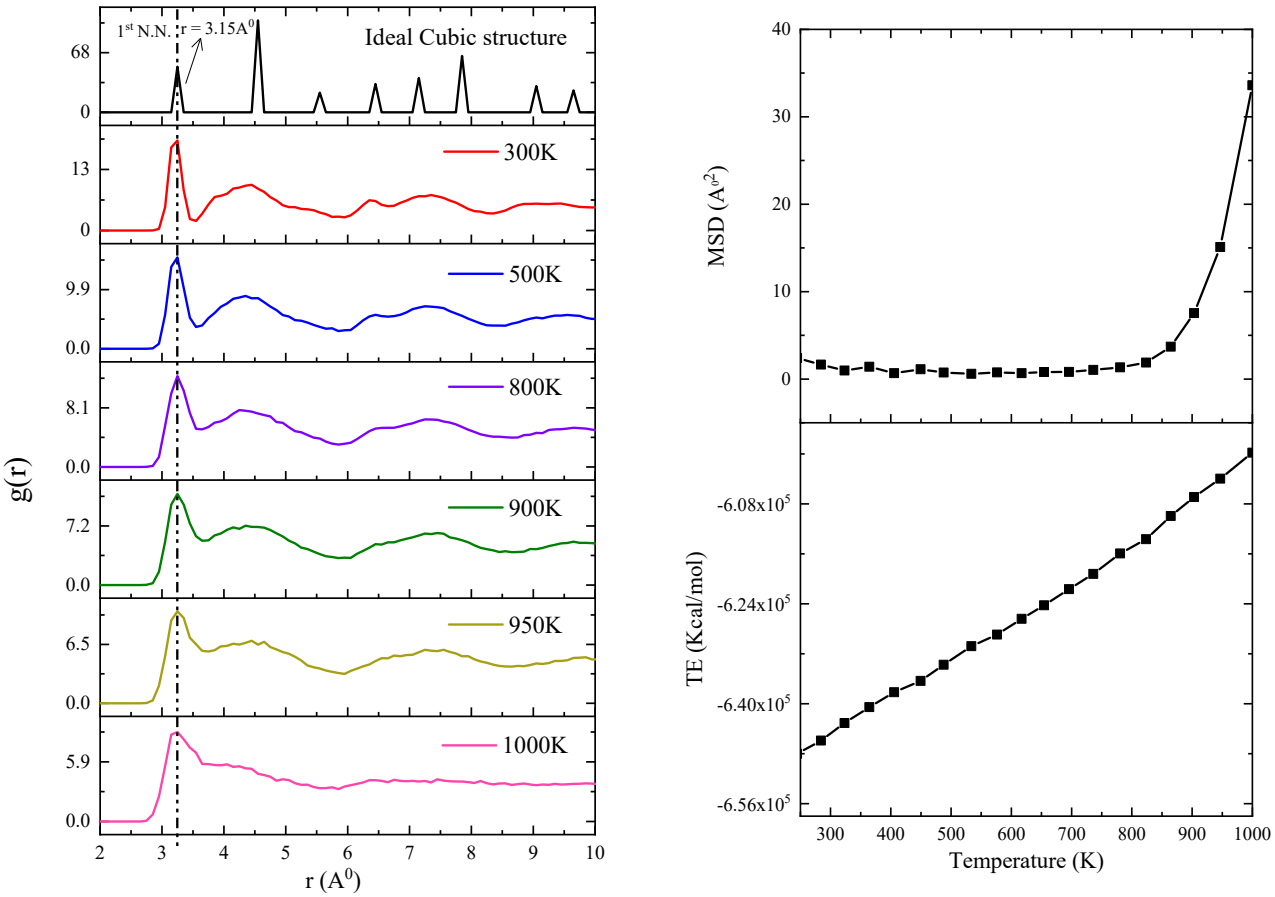
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

[Supporting information]

Mechanical-Load and Temperature-Engendered Degradation of α-$CsPbI_3$: Reactive Molecular Dynamics Simulation

Sunil Kumar*, Trilochan Mishra and Ranjan K. Sahu#
CSIR-National Metallurgical Laboratory, Jamshedpur 831007
[*sunil@nmlindia.org, #rksahu@nmlindia.org]



(a) (b)

Figure 1S Variation in (a) radial density distribution, (b) mean square displacement and total energy of α-$CsPbI_3$ during a gradual heating process (from T=300K to 1000K).

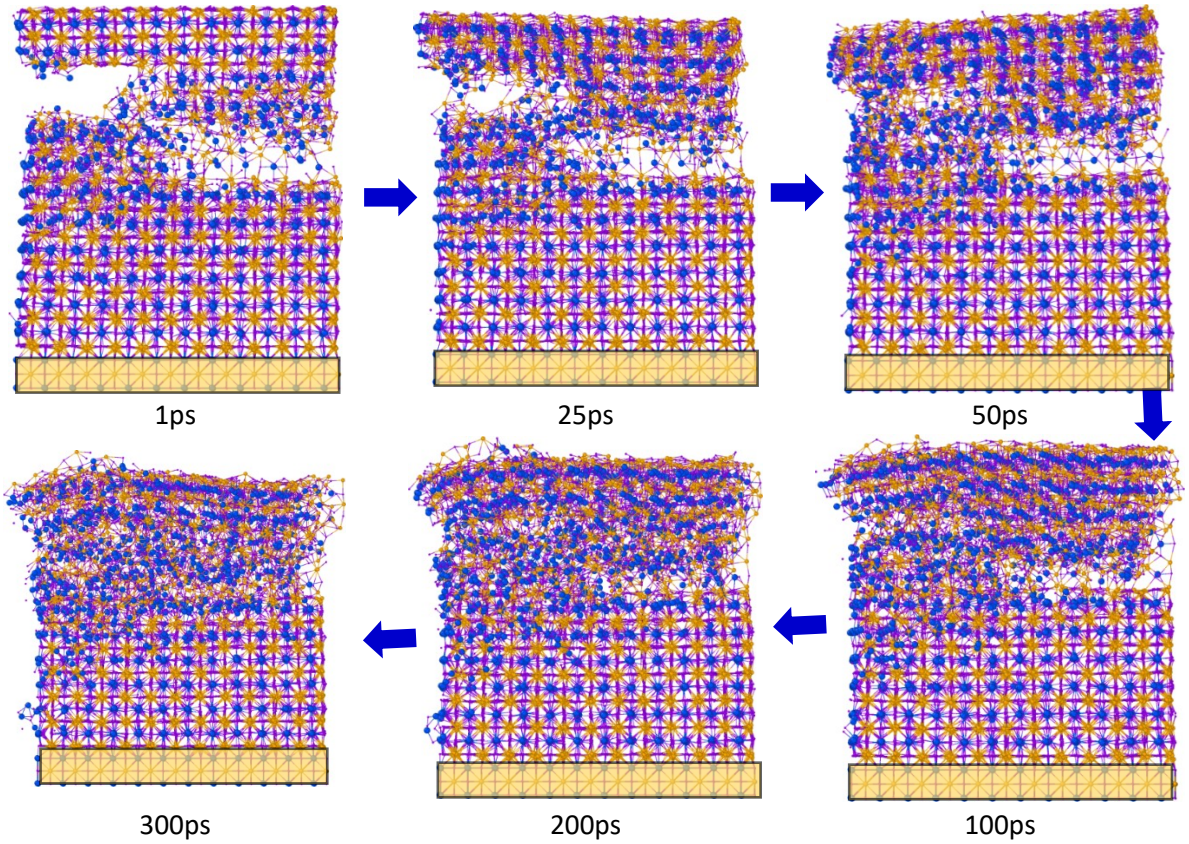


Figure 2S Snapshots of α-$CsPbI_3$ at different times during the relaxing stage. Cs, Pb, and I atoms are represented by blue, yellow, and purple atoms, respectively. The progress of simulation is depicted by blue color arrow.

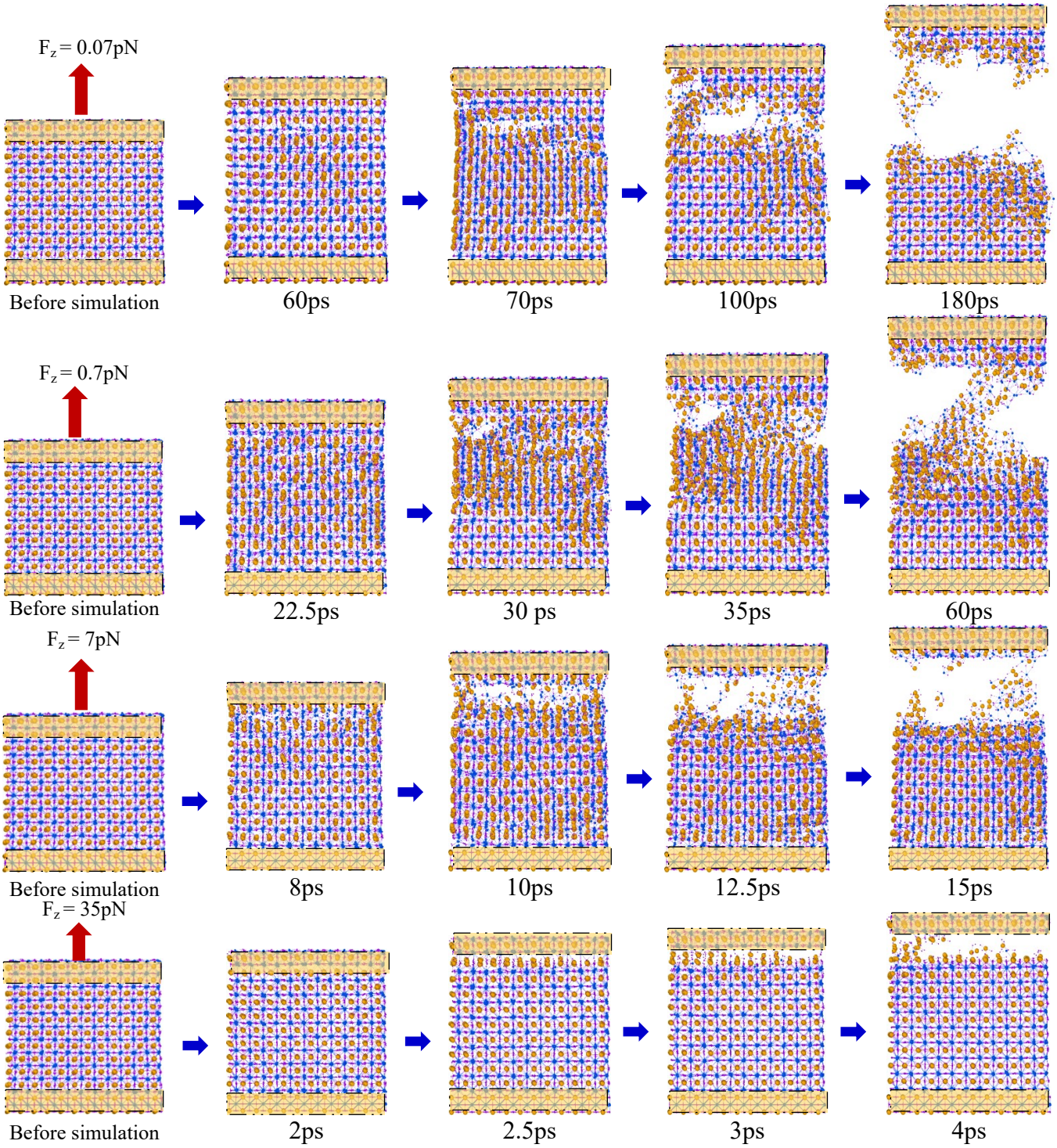


Figure 3S Snapshots of α-$CsPbI_3$ at different times during deformation by a pulling force of magnitude F_z = 0.07pN, 0.7pN, 7pN, and 35pN. Cs, Pb, and I are represented by blue, yellow, and purple atoms, respectively. The direction of the pulling force and the progress of simulation are represented by red and blue color arrows.

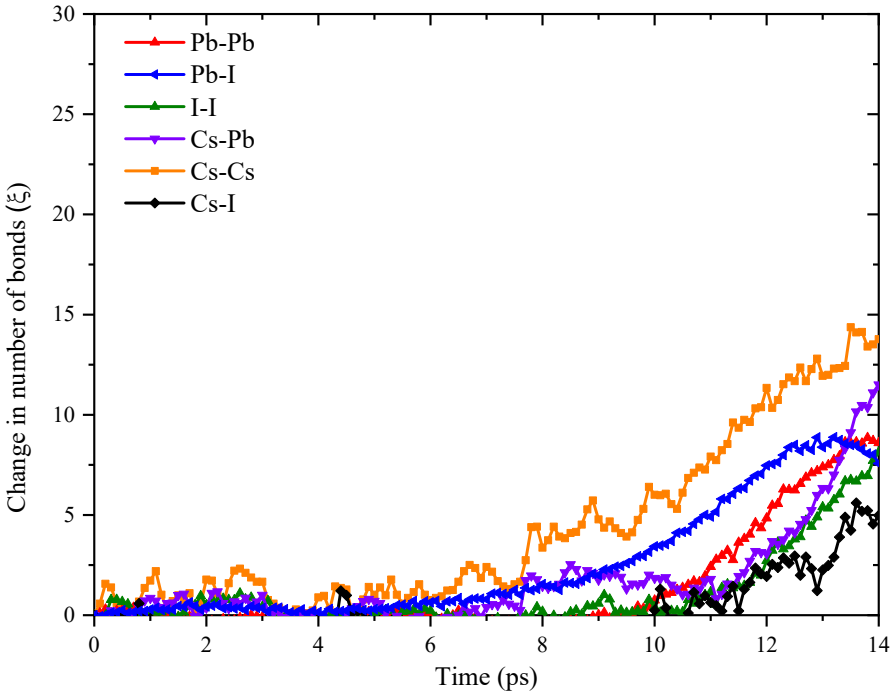


Figure 4S Variation of the percentage change in the number of bonds, α-$CsPbI_3$ during deformation at F_z = 1.74pN and T=300K using cutoff distance ±10% of 1 Nearest Neighbour of Cs.

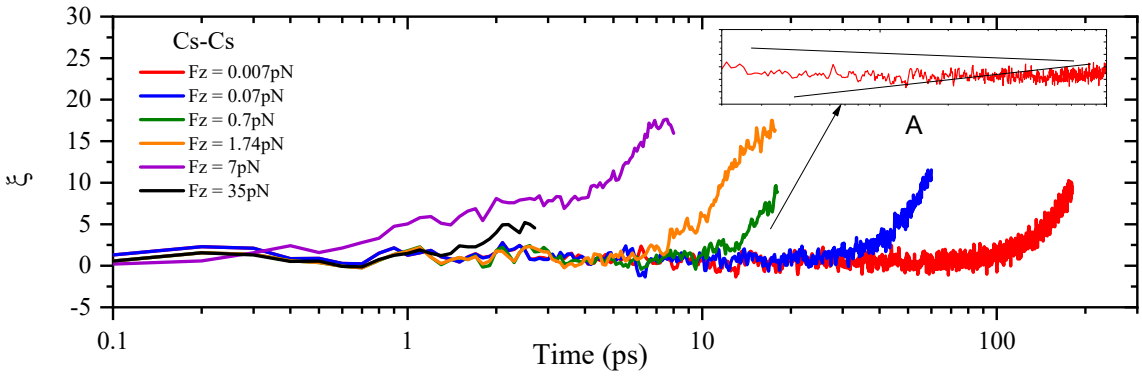


Figure 5S shows the percentage change in the number of bonds of Cs-Cs in α-$CsPbI_3$ using cutoff distance ±10% of 1 Nearest Neighbour of Cs during deformation under a wide range of applied force .

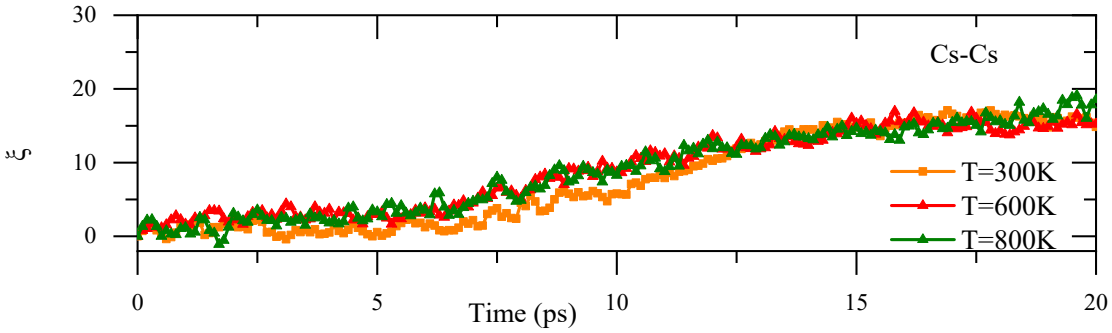
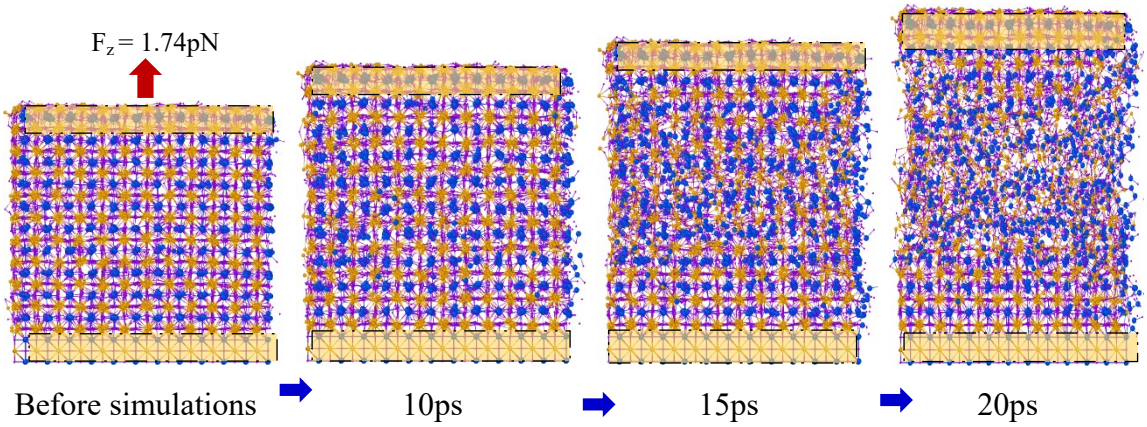
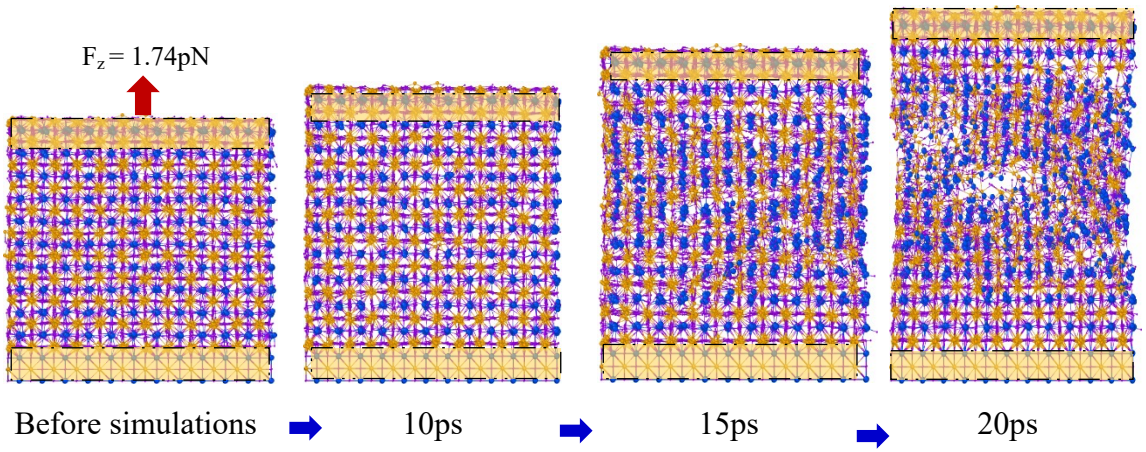


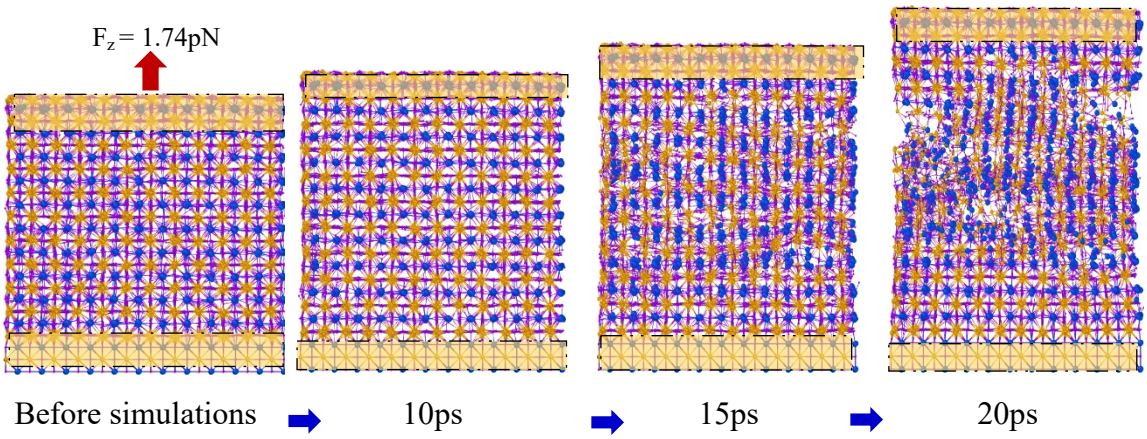
Figure 6S shows the percentage change in the number of bonds of Cs-Cs in α-$CsPbI_3$ using cutoff distance ±10% of 1 Nearest Neighbour of Cs during deformation under a wide range of temperature.



(a)T=800K

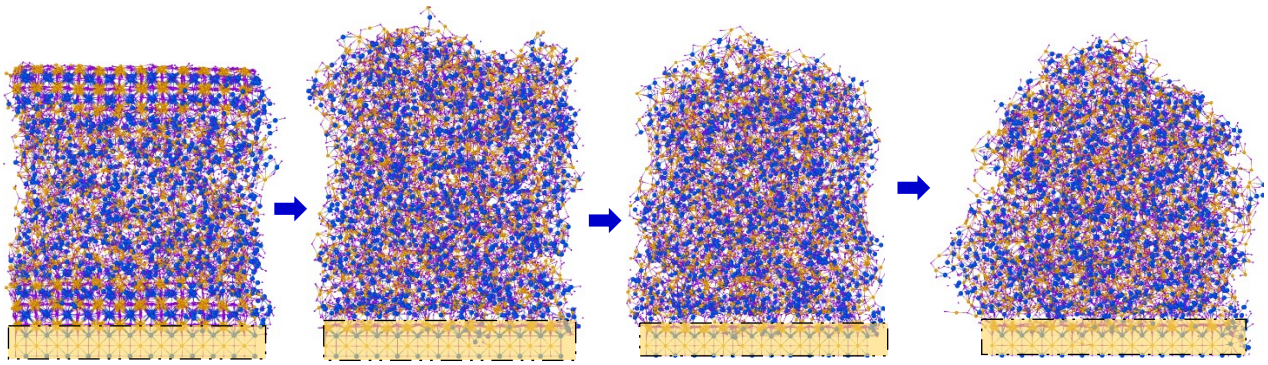


(b)T=600K

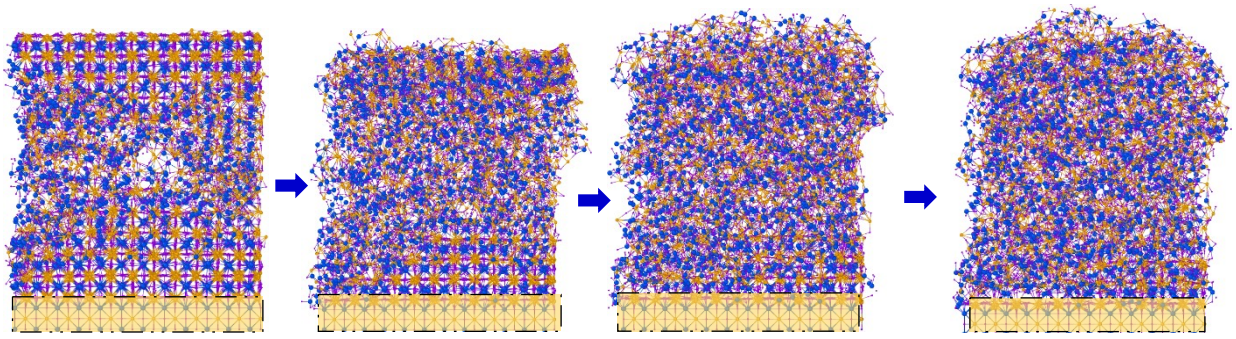


(c)T=400K

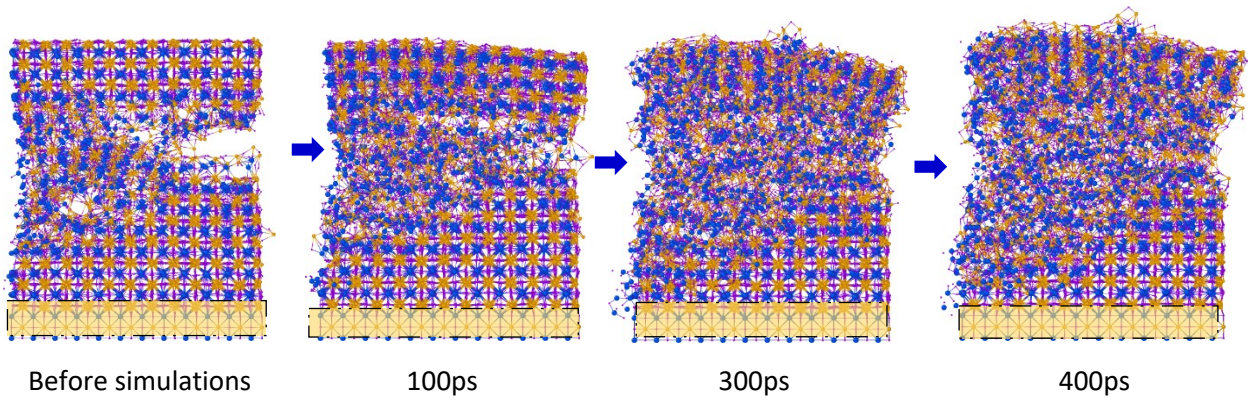
Figure 7S Snapshots of α-$CsPbI_3$ during deformation by a pulling force of magnitude F_z = 1.74pN at various temperatures: (a) 800K, (b) 600K, and (c) 400K. Cs, Pb, and I are represented by blue, yellow, and purple atoms, respectively. The direction of the pulling force and the progress of simulation are represented by red and blue color arrows.



(a)T=800K



(b)T=600K



(c)T=400K

Figure 8S Snapshots of α-$CsPbI_3$ deformed by a pulling force of magnitude Fz = 1.74pN at different temperatures: (a) T=800K, (b) 600K, and (c) 400K. Cs, Pb, and I are represented by blue, yellow, and purple atoms, respectively. The blue color arrow represents the direction of the pulling force and the simulation's progress.