

Supporting Information

Flexible Doorway Controlled Na⁺ Ion Diffusion in NaPSO Glassy Electrolytes from Machine-Learning Force Field Simulations

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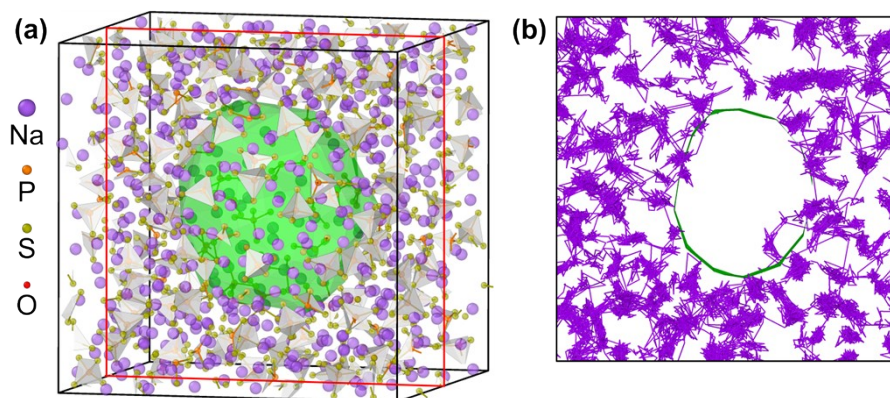


Figure S1. (a) The structure of porous Na_3PS_4 featured a central void (green) with a diameter of approximately 1.4 nm at 300 K. (b) A slice of the porous structure (a) highlighted in red rectangular shows that there are no diffusion trajectories (purple line) passing through the central void at 423 K. The green circle represents the boundary of the void.

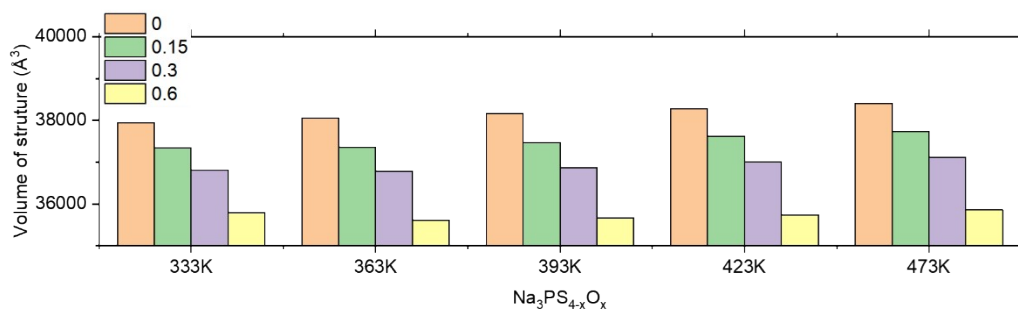


Figure S2. Volume of $\text{Na}_3\text{PS}_{4-x}\text{O}_x$ ($x = 0, 0.15, 0.30,$ and 0.60) supercells with a total of 1600 atoms at various temperatures from 333 K to 473 K.

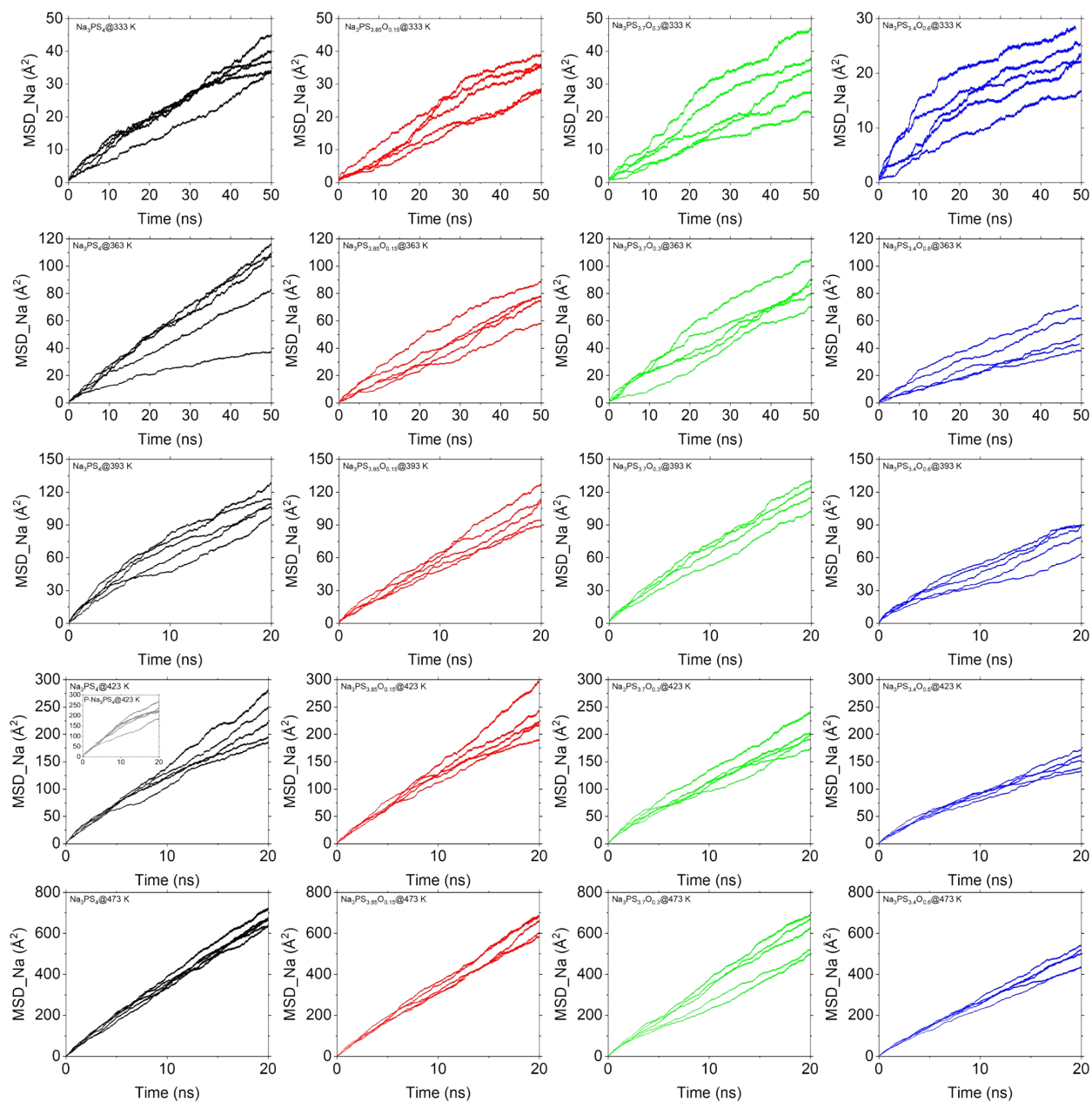


Figure S3. MSD plots of Na-ion diffusion in glassy Na₃PS_{4-x}O_x (x = 0, 0.15, 0.30, and 0.60) at 333K, 363K, 393K, 423K, and 473K.

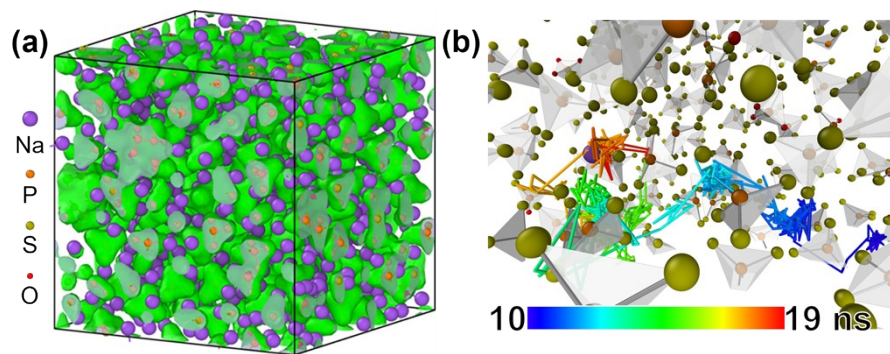


Figure S4. (a) The characteristic feature of the glassy $\text{Na}_3\text{PS}_{3.85}\text{O}_{0.15}$ is that Na ions are distributed within the interstices of the network formed by $\text{PS}_{4-x}\text{O}_x$ clusters (green). (b) The diffusion pathways for Na ions primarily involve shuttling between $\text{PS}_{4-x}\text{O}_x$ clusters within the glassy matrix over the period from 10-19 ns at 423 K.