Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Electronic Supplementary Information (ESI) for:

A Comprehensive Investigation of $Ag_7P_3X_{11}$ (X = O, S, and Se) Solid-State Silver Superionic Conductors.

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† Electronic Supplementary Information (ESI) available: Thermal stability at 300 K for $Ag_7P_3X_{11}$ (X ={ O, S and Se}) structures, Table of decomposition energy, The Radial Distribution Function, The snapshots of AIMD simulation and also the energy profiles(NEB). See DOI: 00.0000/00000000.

Supplementary Note:

1. Stability

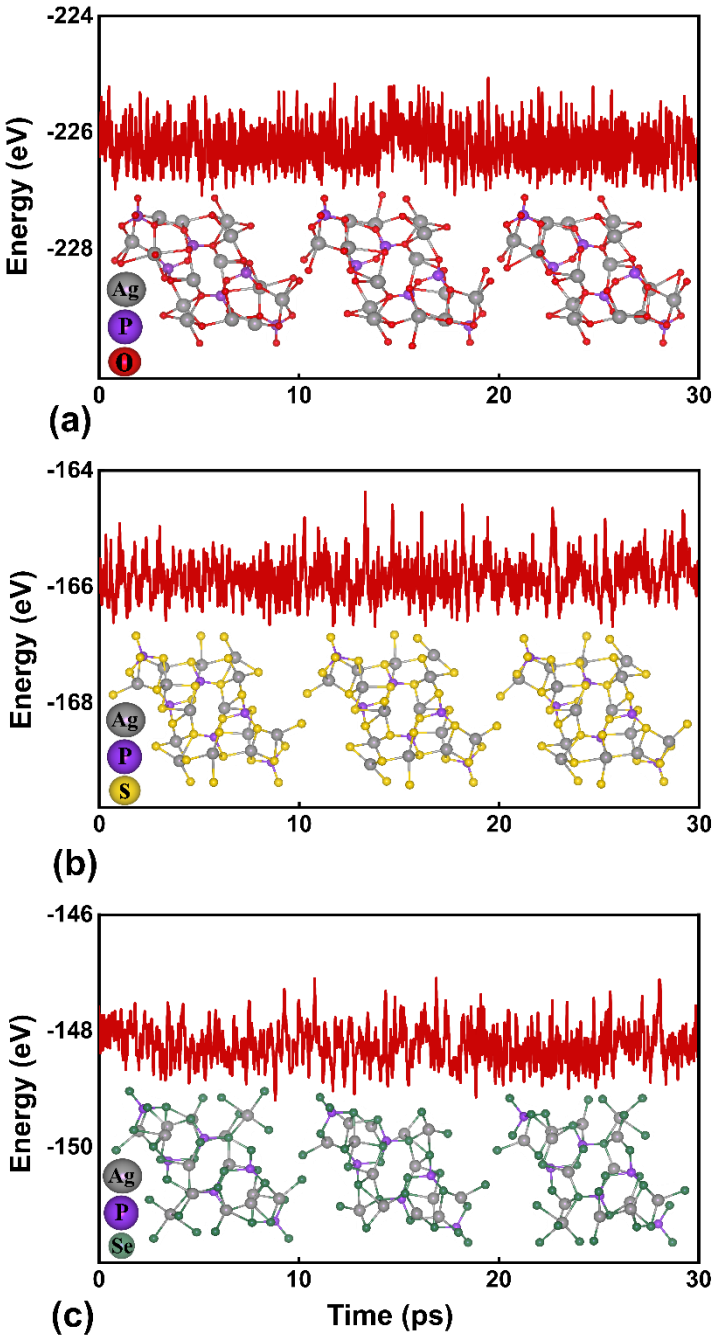

Figure S1. Investigation of thermal stability at 300 K. Energy variation as a function of time for (a) $Ag_7P_3O_{11}$, (b) $Ag_7P_3S_{11}$, (c) $Ag_7P_3Se_{11}$. Snapshots in each 10 ps are shown for each structure.

Table S1. Possible decomposition reactions and the corresponding energies for $Ag_7P_3X_{11}$ (X = O, S, and Se).

Composition	$E_{decomposition}$ (meV/atom)	Possible decomposition reactions
$Ag_7P_3O_{11}$	-4.02	$Ag_3PO_4 + Ag4P_2O_7$
	-8.58	$Ag_3PO_4 + AgPO_3$
	-23.85	$Ag_3PO_4 + P_2O_5$
	-71.93	$Ag_3PO_4 + PO_2+O_2$
	-127.67	$Ag_3PO_4 + P_2O_3+O_2$
$Ag_7P_3S_{11}$	6.43	$Ag_3PS_4 + Ag_4P_2S_7$
	6.31	$Ag_3PS_4 + AgPS_3$
	2.76	$Ag_3PS_4 + P_2S_5$
	-1.11	$Ag_3PS_4 + P_2S_3+S$
	71.21	$Ag_3PS_4 + PS+S$
	-15.40	$Ag_3PS_4 + P_2S+S$
$Ag_7P_3Se_{11}$	-16.56	$Ag_3PSe_4 + Ag_4P_2Se_7$
	0.54	$Ag_3PSe_4 + AgPSe_3$
	13.52	$Ag_3PSe_4 + P_2Se_5$
	18.87	$Ag_3PSe_4 + PSe+Se$
	11.22	$Ag_3PSe_4 + P_2Se+Se$

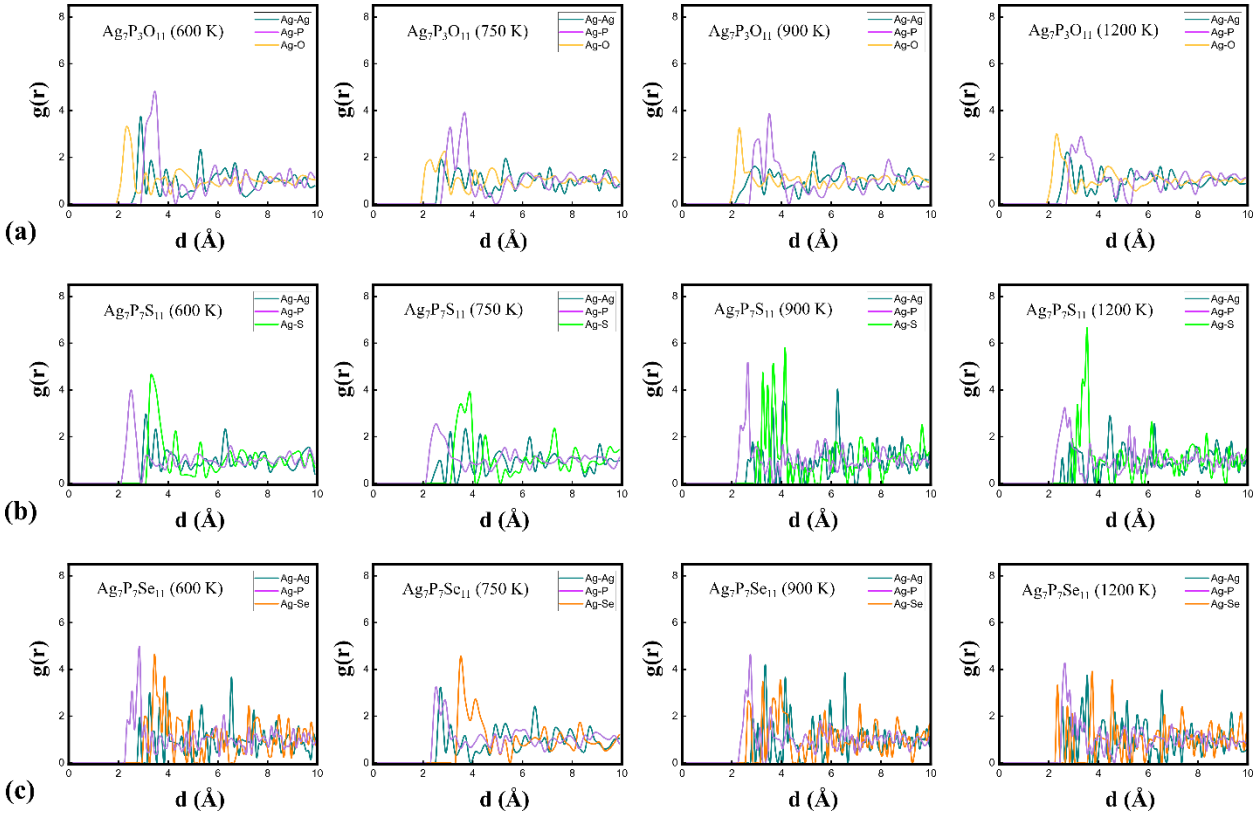

Figure S2. The radial distribution function g(r) at various temperatures (600 K, 750 K, 900 K, and 1200 K) for (a) $Ag_7P_3O_{11}$, (b) $Ag_7P_3S_{11}$ and (c) $Ag_7P_3Se_{11}$.

2. Ionic Conductivity and Diffusivity

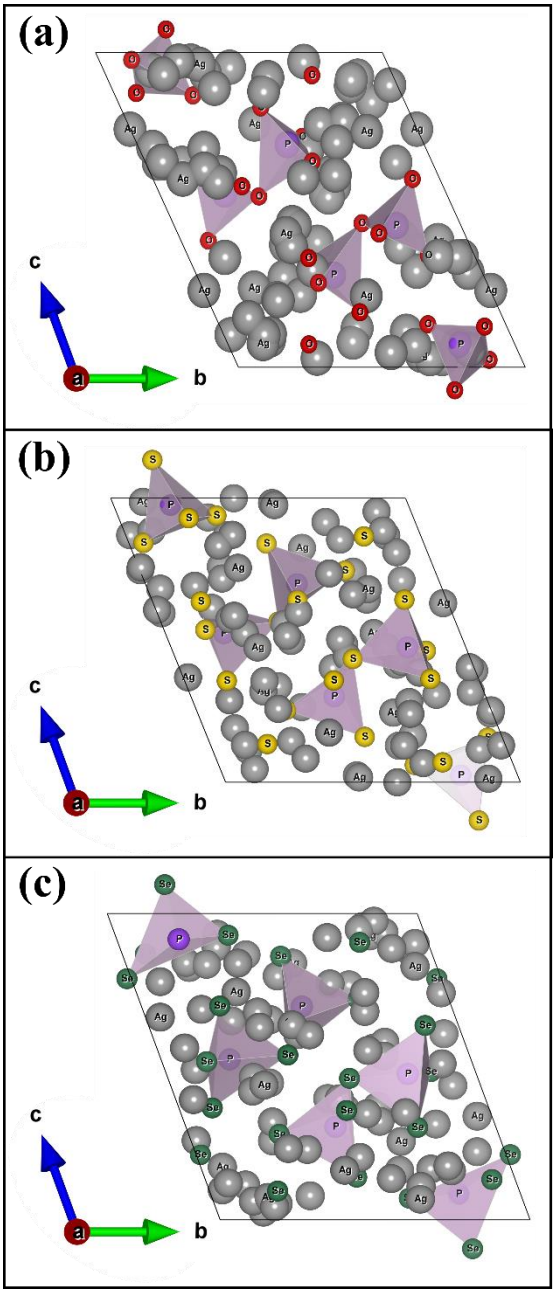

Figure S3. Structural snapshots of AIMD simulation of Ag^{+} ion diffusion at 1200 K at 45 ps for (a) $Ag_7P_3O_{11}$, (b) $Ag_7P_3S_{11}$ and (c) $Ag_7P_3Se_{11}$.

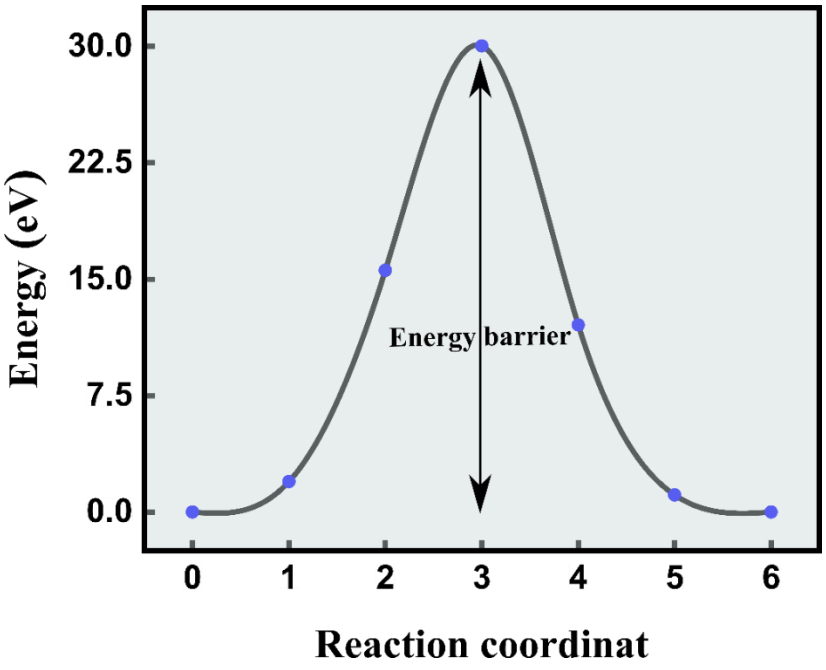

Figure S4. The energy barrier for the reaction paths of Ag^{+} ion migration, obtained by using nudged elastic band (NEB) method for $Ag_7P_3S_{11}$ composition.