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Electronic Supplementary Information

"Defect Chemistry of Disordered Solid-State Electrolyte $Li_{10}GeP_2S_{12}$"

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Phase Stability of $Li_{10}GeP_2S_{12}$ in Chemical Potential Space

The phase stability region of $Li_{10}GeP_2S_{12}$ is calculated from the DFT total energies of competing phases and reference chemical potentials μ^0_{Li} = -1.58 eV, μ^0_{Ge} = -4.34 eV, μ^0_P = -5.14 eV, and μ^0_S = -4.01 eV.

Table S1: Phase stability region of $Li_{10}GeP_2S_{12}$ in the quaternary Li-Ge-P-S chemical potential space.

Corner	$\Delta\mu_{Li}$ (eV)	$\Delta\mu_{Ge}$ (eV)	$\Delta\mu_P$ (eV)	$\Delta\mu_S$ (eV)	Phases in Equlibrium with $Li_{10}GeP_2S_{12}$
P-1	-2.528	-1.509	-1.634	0.000	S, GeS_2, Li_4GeS_4
P-2	-2.530	-1.509	-1.627	0.000	S, GeS_2, Li_3PS_4
P-3	-2.396	-2.046	-2.030	0.000	S, Li_2S, Li_3PS_4
P-4	-2.396	-2.040	-2.033	0.000	S, Li_2S, Li_4GeS_4
P-5	-2.171	-0.427	-0.186	-0.629	LiP_7, GeP_3, Li_3PS_4
P-6	-2.166	-0.424	-0.187	-0.634	LiP_7, GeP_3, Li_4GeS_4
P-7	-2.245	-0.371	-0.204	-0.569	GeS_2, GeP_3, Li_3PS_4
P-8	-2.243	-0.366	-0.206	-0.571	GeS_2, GeP_3, Li_4GeS_4
P-9	-2.031	-0.587	-0.206	-0.729	Li_2S, LiP_7, Li_3PS_4
P-10	-2.030	-0.579	-0.206	-0.731	Li_2S, LiP_7, Li_4GeS_4

Effect of P_{Ge} Anti-Site Defects on the Local Structure

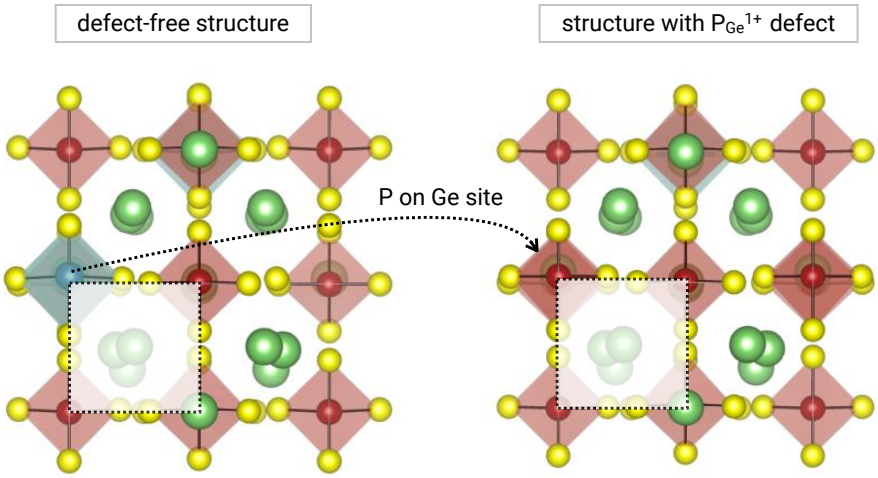

Figure S1: Effect of P_{Ge} anti-site defect on the local structure of LGPS.