Cation-Mutation Design of Quaternary Nitride Semiconductors lattice-matched to GaN

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Table S1. Space group and formation energies ΔH_f (in eV/formula unit) of all the nitride secondary phases.

	Space Group	**ΔH_f**
Ge_3N_4	*P*31*c*	-0.39
Cu_3N	*Pm*-3*m*	-0.02
CuN_3	*I*4$_1$/*amd*	1.887
CuN_6	*Pmcn*	4.07
CuN	*F*-43*m*	1.553
GaN	*P*6$_3$*mc*	-0.972
AlN	*P*6$_3$*mc*	-2.829
InN	*P*6$_3$*mc*	0.158
Li_3N	*P*6/*mmm*	-1.48
LiN_3	*C*2/*m*	-0.587
NaN_3	*R*-3*m*	-0.48
Na_3N	*Pm*-3*m*	0.897
KN_3	*I*4/*mcm*	-0.661
K_3N	*P*6$_3$/*mcm*	1.891
AgN_3	*Ibam*	2.44
Li_5GeN_3	*P*1	-4.453
Li_3GaN_2	*Ia*-3	-3.232
$NaGe_2N_3$	*Cmc*2$_1$	-1.326
Li_3AlN_2	*Ia*-3	-5.128
$LiGe_2N_3$ (never reported)	*Cmc*2$_1$	-2.054

Table S2. Space group and formation energies ΔH_f (in eV/formula unit) of all the non-nitride secondary phases.

	Space Group	**ΔH_f (eV/unit)**
Li_9Ge_4	*Cmcm*	-4.522
Li_3Ge	*Fm*-3*m*	-1.311
$Li_{15}Ge_4$	*I*-43*d*	-6.199
$Li_{11}Ge_6$	*Ccmm*	-5.552
Li_7Ge_2	*Cmmm*	-2.885
LiGe	$I4_1/a$	-0.567
LiGa	*Fd*-3*m*	-0.649
Li_3Ga_2	*R*-3*m*	-1.601
Li_2Ga	*Cmcm*	-0.899
Li_3Ga_7	*R*-3*m*	-2.129
$LiGa_3$	*Pm*-3*m*	-0.732
$L_{i3}Al_2$	*R*-3*m*	-0.907
LiAl	*Fd*-3*m*	-0.359
Li_9Al_4	*C*2/*m*	-2.027
$LiAl_3$	*Pm*-3*m*	-0.325
Li_3In_2	*R*-3*m*	-1.513
Li_2In	*Cmcm*	-0.889
LiIn	*Fd*-3*m*	-0.535
Li_3In	*Fm*-3*m*	-0.988
$Li_{13}In_3$	*Fd*-3*m*	-3.368
$LiIn_3$	*Pm*-3*m*	-0.56
LiGaGe	$P6_3mc$	-0.806
LiAlGe	*F*-43*m*	-0.885
LiInGe	*F*-43*m*	-0.726