ARTICLE

Supporting Information

Ab initio exploration and prediction of *AE*-containing nitrido(litho/magneso)tetrelates (*AE* = Ca, Sr; *Tt* = Si, Ge) with $[Si_2N_6]^{10-}$ or $[Ge_2N_6]^{10-}$-units

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Electronic Structure Calculations

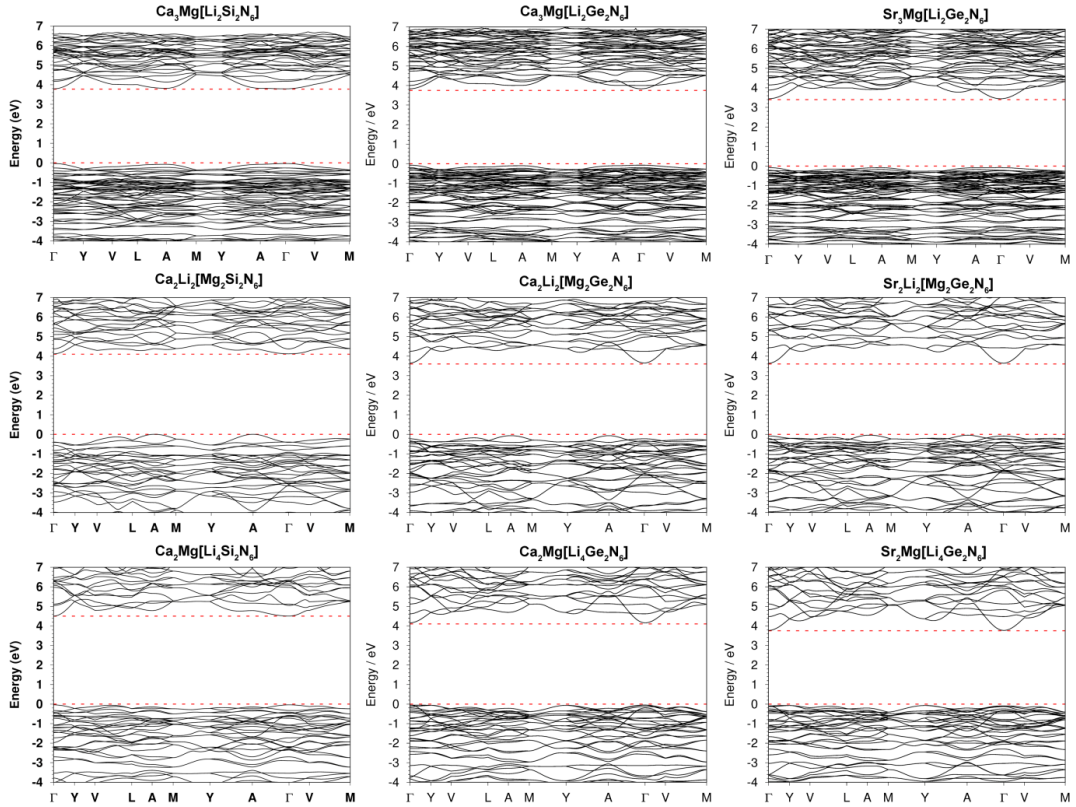

Figure S1 Band structure calculations along high symmetry directions for the studied nitridosilicates and nitridogermanates as calculated within the VASP program with PBEsol in conjunction with the mBJ exchange potential (PBEsol+mBJ).

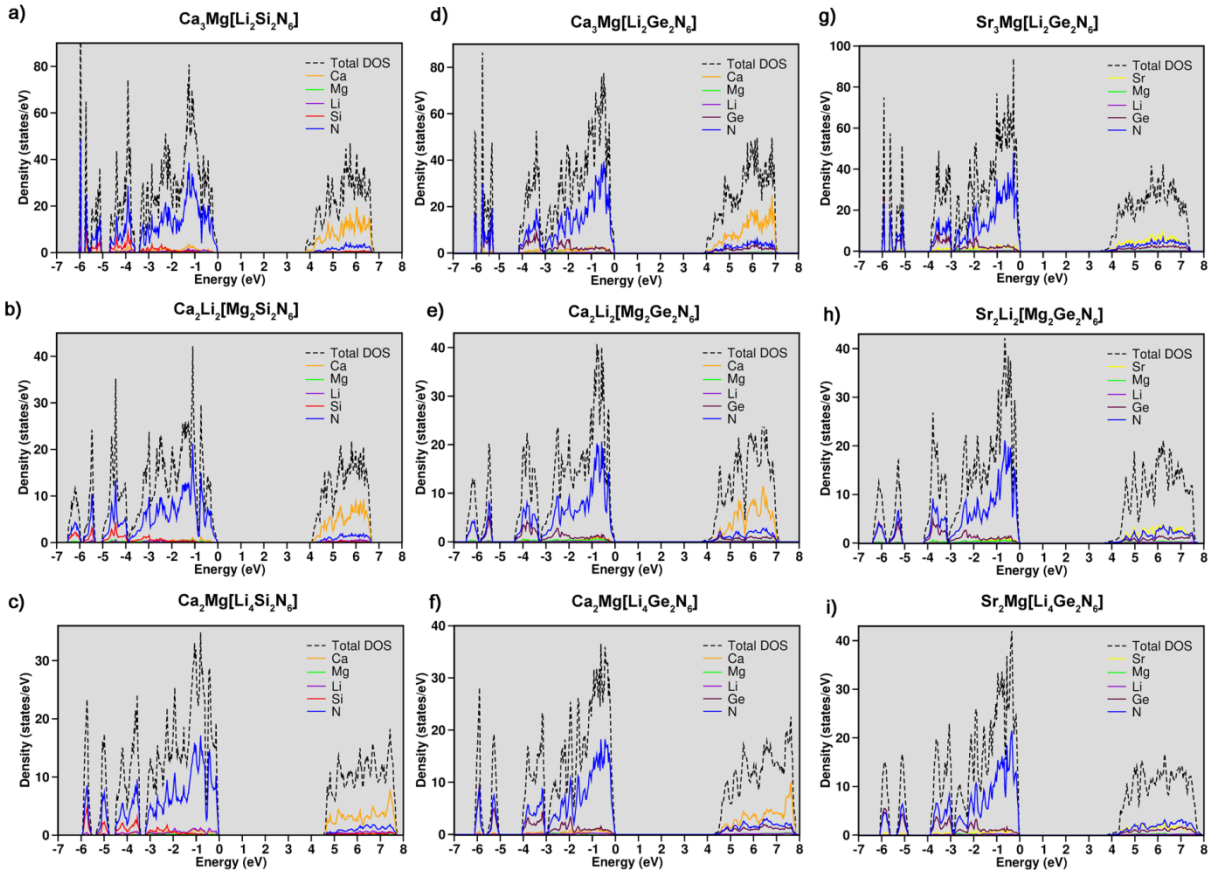

Figure S2 Total and atomic resolved electronic density of states for existing and predicted (litho/magneso)nitridotetrelates (a-i), as calculated within the VASP program with PBEsol in conjunction with the mBJ exchange potential (PBEsol+mBJ).

Absorption Spectra

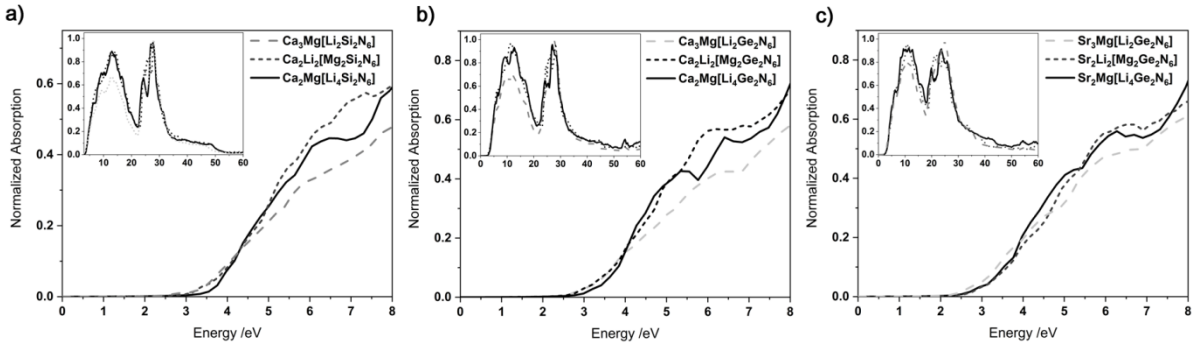

Figure S3 Calculated onset of optical absorption for the studied (litho/magneso)nitridotetrelates as calculated by VASP with PBEsol.

Crystallographic data obtained by structure relaxations and phonon calculations

Table S1. Atomic coordinates, isotropic displacement parameters [Å^2] and site occupancies of $Ca_3Mg[Li_2Ge_2N_6]$, as calculated by DFT calculations.

Atom		*x*	*y*	*z*	U_{eq}	s.o.f
Ca1	8*j*	0.0549	0.3221	0.2469	0.00803	1
Ca2	4*h*	0.0000	0.1784	0.5000	0.01853	1
Ge1	4*i*	0.3518	0	0.4160	0.0052	1
Ge2	4*i*	0.6987	0	0.0644	0.00453	1
Mg	4i	0.0768	0	0.2183	0.00903	1
Li	8j	0.1747	0.1785	0.0616	0.01213	1
N1	8j	0.2305	0.1508	0.3474	0.00876	1
N2	8*j*	0.8579	0.8498	0.1201	0.00643	1
N3	4*i*	0.3199	0	0.5755	0.01013	1
N4	4*i*	0.3840	0	0.0992	0.00653	1

Table S2. Anisotropic displacement parameters of $Ca_3Mg[Li_2Ge_2N_6]$, as calculated by DFT calculations, extrapolated to 300 K by PHONOPY.

Atom	U_{11} /Å^2	U_{22}/ Å^2	U_{33}/ Å^2	U_{12}/ Å^2	U_{13}/ Å^2	U_{23}/ Å^2
Ca1	0.00760	0.00670	0.00980	0.00170	0.00380	0.00230
Ca2	0.02290	0.01470	0.01800	0.00000	0.01500	0.00000
Ge1	0.0057	0.0048	0.0051	0	0.0006	0
Ge2	0.0046	0.0041	0.0049	0	0.0006	0
Mg	0.0099	0.0065	0.0107	0	-0.0033	0
Li	0.0131	0.0114	0.0119	-0.0012	0.0036	-0.0016
N1	0.0089	0.0084	0.009	0.0027	0.0029	0.0031
N2	0.0063	0.0052	0.0078	0.0005	0.0009	0.0006
N3	0.0071	0.0161	0.0072	0	0.0025	0
N4	0.0063	0.0073	0.006	0	0.0011	0

Table S 3. Atomic coordinates, isotropic displacement parameters [Å^2] and site occupancies of $Sr_3Mg[Li_2Ge_2N_6]$, as calculated by DFT calculations.

Atom		*x*	*y*	*z*	U_{eq}	s.o.f
Sr1	8*j*	0.0587	0.3264	0.2436	0.0077	1
Sr2	4*h*	0	0.1807	0.5	0.012	1
Ge1	4*i*	0.3520	0	0.4146	0.00476	1
Ge2	4*i*	0.701	0	0.0611	0.0048	1
Mg	4i	0.743	0	0.2168	0.00973	1
Li	8j	0.1753	0.1761	0.0576	0.01466	1
N1	8j	0.2286	0.1443	0.344	0.00873	1
N2	8*j*	0.8622	0.1466	0.1149	0.00693	1
N3	4*i*	0.3295	0	0.5673	0.01063	1
N4	4*i*	0.3934	0	0.093	0.00726	1

Table S4. Anisotropic displacement parameters of $Sr_3Mg[Li_2Ge_2N_6]$, as calculated by DFT calculations, extrapolated to 300 K by PHONOPY.

Atom	U_{11} /Å^2	U_{22}/ Å^2	U_{33}/ Å^2	U_{12}/ Å^2	U_{13}/ Å^2	U_{23}/ Å^2
Sr1	0.0077	0.0066	0.0088	0.0019	0.0032	0.0025
Sr2	0.0106	0.0146	0.0108	0	0.0054	0
Ge1	0.0051	0.0046	0.0046	0	0.0004	0
Ge2	0.0054	0.0045	0.0045	0	-0.0001	0
Mg	0.0106	0.007	0.0116	0	-0.0041	0
Li	0.0171	0.0152	0.0117	-0.0004	0.0035	-0.0018
N1	0.0095	0.0078	0.0089	-0.0027	0.0023	-0.0029
N2	0.0072	0.006	0.0076	-0.0009	0.0005	-0.0009
N3	0.0064	0.019	0.0065	0	0.0017	0
N4	0.0081	0.0079	0.0058	0	-0.0004	0

Table S5. Atomic coordinates, isotropic displacement parameters [Å^2] and site occupancies of $Sr_2Li_2[Mg_2Ge_2N_6]$, as calculated by DFT calculations.

Atom		*x*	*y*	*z*	U_{eq}	s.o.f
Sr	4*g*	-0.5	-0.3157	0	0.00863	1
Ge	4*i*	0.1277	-0.5	0.1887	0.004333	1
Mg	4*h*	-0.5	-0.241	0.5	0.0064	1
Li	4*i*	-0.3035	-0.5	0.4130	0.01623	1
N1	8*j*	-0.2579	-0.1494	0.3244	0.00883	1
N2	4*i*	-0.1994	-0.5	0.1098	0.00840	1

Table S6. Anisotropic displacement parameters of $Sr_2Li_2[Mg_2Ge_2N_6]$, as calculated by DFT calculations, extrapolated to 300 K by PHONOPY.

Atom	U_{11} /Å^2	U_{22}/ Å^2	U_{33}/ Å^2	U_{12}/ Å^2	U_{13}/ Å^2	U_{23}/ Å^2
Sr	0.0072	0.0105	0.0082	0	0.0023	0
Ge	0.0048	0.0044	0.0038	0	0.0003	0
Mg	0.0064	0.0063	0.0065	0	0.0015	0
Li	0.0206	0.0177	0.0104	0	0.0025	0
N1	0.0089	0.0083	0.0093	0.0025	0.0028	0.0042
N2	0.0055	0.0146	0.0051	0	0.0009	0

Table S7. Atomic coordinates, isotropic displacement parameters [Å^2] and site occupancies of $Sr_2Mg[Li_4Ge_2N_6]$, as calculated by DFT calculations.

Atom		*x*	*y*	*z*	U_{eq}	s.o.f
Sr	4*g*	0.5	0.1759	0	0.00956	1
Ge	4*i*	0.3113	0	0.3696	0.00930	1
Mg	2*a*	0	0	0	0.03143	1
Li	8*j*	0.1608	0.1703	0.6226	0.02046	1
N1	4*i*	0.6271	0	0.3075	0.01183	1
N2	*8j*	0.1613	0.1462	0.2537	0.01140	1

Table S8. Anisotropic displacement parameters of $Sr_2Mg[Li_4Ge_2N_6]$, as calculated by DFT calculations, extrapolated to 300 K by PHONOPY.

Atom	U_{11} /Å^2	U_{22}/ Å^2	U_{33}/ Å^2	U_{12}/ Å^2	U_{13}/ Å^2	U_{23}/ Å^2
Sr	0.0079	0.0065	0.0143	0	0.0049	0
Ge	0.0091	0.0054	0.0134	0	0.004	0
Mg	0.0303	0.0078	0.0562	0	-0.0255	0
Li	0.0155	0.023	0.0229	0.0020	0.0051	-0.0066
N1	0.0125	0.0082	0.0148	0	0.0027	0
N2	0.0093	0.0072	0.0177	0.0012	0.0046	0.0012