Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A Novel Class of Multivalent Ionic Conductors of the La_3CuSiS_7 Structure Type: the Results of Stepwise ICSD Screening

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Supplementary information

Table S1. Previously reported Mg^{2+}-, Ca^{2+}-, Zn^{2+}-, Al^{3+}-ionic conducting chalcogenides, on the basis of which the criteria for the GT analysis were parametrized.

WI	Environmental anion	Conductor	Reference
Mg^{2+}	S^{2-}	$Mg_2Mo_6S_8$	DOI: 10.1038/35037553, DOI: 10.1103/PhysRevB.67.104103, DOI: 10.1002/adma.200701495
		$Mg_{0.224}TiS_2$	DOI: 10.1021/acs.chemmater.8b00552, DOI: 10.1021/acs.chemmater.7b04406
		$MgCo_2S_4$	DOI: 10.1039/C6CP08284J
		$MgCr_2S_4$	Patent: US9077032B2, DOI: 10.1021/acs.inorgchem.8b01417, DOI: 10.1039/C6CP08284J
		$MgFe_2S_4$	DOI: 10.1039/C6CP08284J
		$MgIn_2S_4$	DOI: 10.1038/s41467-017-01772-1
		$MgNi_2S_4$	DOI: 10.1039/C6CP08284J
		$MgPS_3$	DOI: 10.1016/j.ssi.2013.10.037
		$MgSc_2S_4$	DOI: 10.1038/s41467-017-01772-1
		$MgMn_2S_4$	DOI: 10.1039/C6CP08284J
		$MgMo_6S_8$	DOI: 10.1021/cm061656f, DOI: 10.1103/PhysRevB.67.104103, DOI: 10.1016/j.jpowsour.2015.12.009
		$MgTi_2S_4$	Link: https://search.proquest.com/docview/2283937545?pq-origsite=gscholar, DOI: 10.1021/acs.chemrev.6b00614, DOI: 10.1039/C6CP08284J
		MgV_2S_4	Link: https://search.proquest.com/docview/2283937545?pq-origsite=gscholar, Patent: US9077032B2
		MgY_2S_4	DOI: 10.1038/s41467-017-01772-1
		$MgLu_2S_4$	DOI: 10.1039/C9CC09510A
		$MgTm_2S_4$	DOI: 10.1039/C9CC09510A
		$MgEr_2S_4$	DOI: 10.1039/C9CC09510A
		$MgHo_2S_4$	DOI: 10.1039/C9CC09510A
		$MgDy_2S_4$	DOI: 10.1039/C9CC09510A
		$MgTb_2S_4$	DOI: 10.1039/C9CC09510A
		$MgSm_2S_4$	DOI: 10.1039/C9CC09510A
		$MgPm_2S_4$	DOI: 10.1039/C9CC09510A
		$MgNd_2S_4$	DOI: 10.1039/C9CC09510A
		$MgPr_2S_4$	DOI: 10.1039/C9CC09510A
		$MgLa_2S_4$	DOI: 10.1039/C9CC09510A
	Se^{2-}	$MgCr_2Se_4$	Patent: US9077032B2, Link: https://search.proquest.com/docview/2283937545?pq-origsite=gscholar
		$MgIn_2Se_4$	DOI: 10.1038/s41467-017-01772-1
		$MgGa_2S_4$	DOI: 10.1021/acsomega.9b00482
		$MgMo_6Se_8$	DOI: 10.1002/adma.200701495, DOI: 10.1016/j.jpowsour.2015.12.009
		$MgSc_2Se_4$	DOI: 10.1038/s41467-017-01772-1
		MgY_2Se_4	DOI: 10.1038/s41467-017-01772-1
		$MgLu_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgTm_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgEr_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgHo_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgDy_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgTb_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgSm_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgPm_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgNd_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgPr_2Se_4$	DOI: 10.1039/C9CC09510A
		$MgLa_2Se_4$	DOI: 10.1039/C9CC09510A
Ca^{2+}	S^{2-}	$CaMo_6S_8$	DOI: 10.1039/C7CP03378H, DOI: 10.1016/j.jpowsour.2015.12.009

		$CaLa_2S_4$	DOI: 10.1016/0025-5408(81)90084-2
		$CaCe_2S_4$	DOI: 10.2320/matertrans1960.22.399
		$Ca_{0.5}TiS_2$	DOI: 10.2320/matertrans1960.22.399, DOI: 10.1021/acs.chemmater.7b04406
Zn^{2+}	S^{2-}	$ZnIn_2S_4$	DOI: 10.1038/s41467-017-01772-1
		$ZnSc_2S_4$	DOI: 10.1038/s41467-017-01772-1
		ZnY_2S_4	DOI: 10.1038/s41467-017-01772-1
		$ZnMo_3S_4$	DOI: 10.1016/0022-4596(87)90179-4
		$ZnPS_3$	DOI: 10.1021/acs.chemmater.9b00207
		$ZnMo_6S_8$	DOI: 10.1016/0022-4596(87)90179-4
	Se^{2-}	$ZnMo_6Se_8$	DOI: 10.1016/0022-4596(87)90179-4
		ZnY_2Se_4	DOI: 10.1038/s41467-017-01772-1
		$ZnSc_2Se_4$	DOI: 10.1038/s41467-017-01772-1
		$ZnIn_2Se_4$	DOI: 10.1038/s41467-017-01772-1
		$Zn_{0.5}Nb_6Se_8$	DOI: 10.1016/0025-5408(87)90261-3
Al^{3+}	S^{2-}	$AlCr_2S_4$	DOI: 10.1039/C6CP08284J
		$AlCo_2S_4$	DOI: 10.1039/C6CP08284J
		$AlNi_2S_4$	DOI: 10.1039/C6CP08284J
		$AlMn_2S_4$	DOI: 10.1039/C6CP08284J
		$Al_{13}Tl_3S_{21}$	DOI: 10.1002/chem.201901438
		$AlPS_4$	DOI: 10.1002/chem.201901438
		$Al_{0.44}La_3Si_{0.93}S_7$	DOI: 10.1002/chem.201901438

Table S2. 24 promising ternary and quaternary Mg-/S(Se,Te)-containing compounds after the GT analysis sorted in ascending order of the migration barrier energy E_m from BVSE. Electronic band gap energies E_g (if any) were taken from https://materialsproject.org. The theoretical gravimetric capacity C_g was calculated for compounds with electrochemically active transition metals (if the compound does not contain a transition metal, it is indicated as a "SE").

Framework type	Chemical formula	Space Group symmetry	GT				E_m(BVSE), eV	E_g, eV	C_g, mAh/g	ρ, g/cm^3	Cv, mAh/ cm^3	*GII*	ICSD-#
			Dimension of migration	Direction of migration	R_{sd}, Å	r_{chan}, Å							
$[M_2E_4]^{2-}$ M=Cr, Yb; E=S, Se, Te	$MgYb_2Se_4$	*Fd*-3*m*	3D	-	2.467	1.828	0.13	0.00	SE	6.083	-	0.29	76053
	$MgYb_2S_4$	*Fd*-3*m*	3D	-	2.267	1.635	0.43	0.00	SE	5.022	-	0.19	642803
$[SnSe_4]^{4-}$	Mg_2SnSe_4	*Pnma*	1D	[010]	2.191	1.704	0.62	1.35	SE	4.729	-	0.57	642819
$[Al_2Se_8]^{10-}$	$Mg_5Al_2Se_8$	*Pna*2$_1$	1D	[001]	2.298	1.712	0.80	-	SE	4.128	-	0.31	100113
$[M_3TE_7]^-$ M=Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er; T=Ge, Si; E=S, Se, Te	$Mg_{0.5}Tb_3GeS_7$	*P*6$_3$	1D	[001]	2.274	1.642	1.02	-	SE	5.425	-	0.11	154786
	$MgLa_6Si_2S_{14}$	*P*6$_3$	1D	[001]	2.043	1.526	1.08	-	SE	4.238	-	0.11	84832
	$Mg_{0.5}Pr_3GeS_7$	*P*6$_3$	1D	[001]	2.009	1.504	1.10	-	SE	4.717	-	0.14	154782
	$MgLa_6Ge_2S_{14}$	*P*6$_3$	1D	[001]	2.015	1.528	1.14	-	SE	4.455	-	0.12	84831
$[M_3ME_7]^{2-}$ M= La, Ce; M=Al; E=S, Se, Te	$MgLa_3AlS_7$	*P*6$_3$	1D	[001]	2.025	1.541	1.17	2.30	SE	4.220	-	0.21	608298
$[M_3TE_7]^-$ M=Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er; T=Ge, Si; E=S, Se, Te	$Mg_{0.5}Ce_3GeS_7$	*P*6$_3$	1D	[001]	2.042	1.513	1.23	-	SE	4.606	-	0.15	240913
$[M_2E_4]^{2-}$ M=Cr, Yb; E=S, Se, Te	**$Mg(Ga_{0.1}Cr_{0.9})_2S_4$**	*Fd*-3*m*	3D	-	1.509	2.087	1.25	1.00	**309**	3.378	1044	0.10	107568
$[ME_4]^{4-}$ M=Si, Ge, Sn; E=S, Se, Te	Mg_2GeS_4	*Pnma*	3D	-	2.061	1.581	1.25	2.31	SE	2.846	-	0.07	636952
$[M_3TE_7]^-$ M=Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er; T=Ge, Si; E=S, Se, Te	$Mg_{0.5}Sm_3GeS_7$	*P*6$_3$	1D	[001]	2.219	1.620	1.29	-	SE	5.089	-	0.11	154784
	$Mg_{0.5}Nd_3GeS_7$	*P*6$_3$	1D	[001]	2.204	1.505	1.32	-	SE	4.834	-	0.12	154783
$[M_3ME_7]^{2-}$ M= La, Ce; M=Al; E=S, Se, Te	$MgCe_3AlS_7$	*P*6$_3$	1D	[001]	2.029	1.523	1.33	0.18	SE	4.333	-	0.11	606475
$[M_3TE_7]^-$ M=Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er; T=Ge, Si; E=S, Se, Te	$Mg_{0.5}Gd_3GeS_7$	*P*6$_3$	1D	[001]	2.191	1.602	1.43	-	SE	5.319	-	0.35	154785
$[ME_4]^{4-}$ M=Si, Ge, Sn; E=S, Se, Te	Mg_2SnS_4	*Pnma*	3D	-	2.094	1.609	1.49	2.13	SE	3.238	-	0.10	243675
	Mg_2SiS_4	*Pnma*	3D	-	2.013	1.551	1.55	2.97	SE	2.436	-	0.13	642791
$[M_3TE_7]^-$ M=Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er; T=Ge, Si; E=S, Se, Te	$Mg_{0.5}Dy_3GeS_7$	*P*6$_3$	1D	[001]	2.173	1.594	1.56	-	SE	5.550	-	0.09	154787
	$Mg_{0.5}Y_3GeS_7$	*P*6$_3$	1D	[001]	2.171	1.594	1.59	-	SE	3.992	-	0.17	154780
	$Mg_{0.5}Er_3GeS_7$	*P*6$_3$	1D	[001]	2.159	1.588	1.67	-	SE	5.707	-	0.17	154789
	$MgY_6Si_2S_{14}$	*P*6$_3$	1D	[001]	2.128	1.565	1.77	-	SE	3.730	-	0.30	642792

	$Mg_{0.5}Ho_3GeS_7$	*P*6$_3$	1D	[001]	2.137	1.579	1.82	-	SE	5.615	-	0.14	154788
$[Al_2S_4]^{2-}$	$MgAl_2S_4$	*R*-3*m*	2D	(001)	2.121	1.510	1.84	2.02	SE	2.438	-	0.19	107308

*Promising cathode materials and corresponding values of their gravimetric capacities are highlighted in bold.

Table S3. 17 promising ternary and quaternary Ca-/S(Se,Te)-containing compounds after the GT analysis sorted in ascending order of the migration barrier energy E_m from BVSE. Electronic band gap energies E_g (if any) were taken from https://materialsproject.org. The theoretical gravimetric capacity C_g was calculated for compounds with electrochemically active transition metals (if the compound does not contain a transition metal, it is indicated as a "SE").

Framework type	Chemical formula	Space Group symmetry	GT				E_m(BVSE), eV	E_g, eV	C_g, mAh/g	ρ, g/cm^3	Cv, mAh/cm^3	*GII*	ICSD-#
			Dimension of migration	Direction of migration	R_{sd}, Å	r_{chan}, Å							
$[K_4Te_3]^-$	$Ca_{0.667}K_4Te_3$	*I*4/*mcm*	1D	[001]	1.988	2.601	0.38	-	SE	3.215	-	0.45	71608
$[In_2Te_4]^{2-}$	$CaIn_2Te_4$	*I*4/*mcm*	1D	[001]	2.099	3.087	0.53	-	SE	5.118	-	0.20	24388
$[Zn_{0.5}Se]^-$	$Ca_{0.5}Zn_{0.5}Se$	*P*-4*m*2	2D	(001)	1.924	2.674	0.76	2.25	SE	3.777	-	0.32	167832
$[Ga_2S_4]^{2-}$	$CaGa_2S_4$	*Cccm*	1D	[100]	1.512	1.474	0.95	2.72	SE	3.343	-	0.25	619292
$[ME_2]^-$ M=Dy, Ho, Er, Lu; E=S, Se, Te	$Ca_{0.5}DyTe_2$	*R*-3*m*	2D	(001)	2.084	2.790	1.61	-	SE	6.085	-	0.94	619251
	$Ca_{0.5}ErTe_2$	*R*-3*m*	2D	(001)	2.079	2.783	1.61	-	SE	6.216	-	1.00	619258
	$Ca_{0.5}LuTe_2$	*R*-3*m*	2D	(001)	2.064	2.741	1.75	-	SE	6.383	-	1.01	619399
	$Ca_{0.5}HoSe_2$	*R*-3*m*	2D	(001)	1.875	2.494	2.06	-	SE	5.757	-	0.19	619371
$[ME_4]^{4-}$ M=Si, Ge, Sn; E=S, Se, Te	Ca_2SnS_4	*Pnma*	1D	[010]	1.655	1.897	2.32	2.30	SE	2.926	-	0.09	429695
$[ME_2]^-$ M=Dy, Ho, Er, Lu; E=S, Se, Te	$Ca_{0.5}HoTe_2$	*R*-3*m*	2D	(001)	1.994	2.651	2.47	-	SE	6.149	-	0.62	619373
$[ME_4]^{4-}$ M=Si, Ge, Sn; E=S, Se, Te	Ca_2SiSe_4	*Pnma*	1D	[010]	1.743	2.401	2.95	2.42	SE	6.585	-	0.42	619574
	Ca_2GeS_4	*Pnma*	1D	[010]	1.627	1.877	2.95	2.56	SE	2.658	-	0.39	619332
	$CaYbInSe_4$	*Pnma*	1D	[010]	1.698	2.409	3.24	0.00	SE	5.358	-	0.09	67654
	Ca_2SiS_4	*Pnma*	1D	[010]	1.607	1.869	3.35	3.11	SE	2.324	-	0.46	619542
$[YbInS_4]^{2-}$	$CaYbInS_4$	*Pnma*	3D	-	1.574	1.904	3.56	0.00	SE	4.310	-	0.09	67655
$[Sc_2S_4]^{2-}$	$CaSc_2S_4$	*Pnma*	1D	[001]	1.634	2.206	4.31	1.29	SE	2.970	-	0.04	27181
$[Y_2S_4]^{2-}$	CaY_2S_4	*Pnma*	1D	[010]	1.473	1.940	4.84	1.54	SE	3.482	-	0.06	619557

Table S4. 28 promising ternary and quaternary Zn-/S(Se,Te)-containing compounds after the GT analysis sorted in ascending order of the migration barrier energy E_m from BVSE. Electronic band gap energies E_g (if any) were taken from https://materialsproject.org. The theoretical gravimetric capacity C_g was calculated for compounds with electrochemically active transition metals (if the compound does not contain a transition metal, it is indicated as a "SE").

Framework type	Chemical formula	Space Group symmetry	Dimension of migration	GT			E_m(BVSE), eV	E_g, eV	C_g, mAh/g	ρ, g/cm^3	Cv, mAh/cm^3	*GII*	ICSD-#
				Direction of migration	R_{sd}, Å	r_{chan}, Å							
[ME4]2- M=Al, Cr, Mn, Ga, In, Yb, Ni, Cr; E=S, Se, Te	$ZnYb_2Se_4$	*Fd*-3*m*	3D	-	1.692	2.020	0.17	0.00	SE	6.521	-	0.23	652208
	$ZnMn_2Se_4$	*Fd*-3*m*	3D	-	1.620	2.254	0.19	0.00	109	5.038	549	0.34	643609
$[M_3TE_7]^{2-}$ M=La, Ce, Gd; T=Al, Ga; E=S, Se, Te	$ZnLa_3GaSe_7$	*P*6$_3$	1D	[001]	1.565	2.014	0.25	-	SE	5.881	-	0.29	431499
[ME4]2- M=Al, Cr, Mn, Ga, In, Yb, Ni, Cr; E=S, Se, Te	**$ZnCr_{1.94}In_{0.06}Se_4$**	*Fd*-3*m*	3D	-	1.577	2.183	0.29	-	**164**	5.608	920	0.19	85040
	$ZnCr_{1.95}Ni_{0.05}Se_4$	*Fd*-3*m*	3D	-	1.576	2.181	0.29	-	**166**	5.586	927	0.46	93392
$[Cl_2S_5]^{12-}$	$Zn_6Cl_2S_5$	*Cmcm*	2D	(100)	1.725	1.910	0.29	-	SE	2.658	-	1.11	419561
[ME4]2- M=Al, Cr, Mn, Ga, In, Yb, Ni, Cr; E=S, Se, Te	**$ZnCr_{1.6}Ga_{0.4}Se_4$**	*Fd*-3*m*	3D	-	1.576	2.186	0.30	-	**163**	5.679	926	0.90	88795
	$ZnCr_2Se_4$	*Fd*-3*m*	3D	-	1.583	2.188	0.31	0.05	**166**	5.552	922	0.05	626760
	$ZnCr_{1.85}Al_{0.15}Se_4$	*Fd*-3*m*	3D	-	1.577	2.183	0.33	-	**167**	5.517	921	0.10	157339
$[Nb_6S_8]^{2-}$	$ZnNb_6S_8$	*P*6$_3$/*m*	1D	[001]	1.955	2.699	0.34	-	122	5.883	718	0.81	645346
$[In_2S_6]^{6-}$	$Zn_3In_2S_6$	*P*3*m*1	2D	(001)	1.577	2.007	0.34	0.00	SE	4.187	-	0.23	68645
[ME4]2- M=Al, Cr, Mn, Ga, In, Yb, Ni, Cr; E=S, Se, Te	**$ZnMn_2S_4$**	*Fd*-3*m*	3D	-	1.525	2.135	0.36	0.00	**176**	3.584	631	0.30	643504
$[M_6T_2S_{14}]^{2-}$ M=La, Y; T=Ge, Si; E=S, Se, Te	$ZnLa_6Ge_2S_{14}$	*P*6$_3$	1D	[001]	1.528	1.905	0.43	-	SE	4.592	-	0.14	636870
	$ZnLa_6Si_2S_{14}$	*P*6$_3$	1D	[001]	1.524	1.943	0.45	-	SE	4.379	-	0.13	641849
$[CaOS]^{2-}$	ZnCaOS	*Cmcm*	2D	(001)	1.582	2.106	0.46	-	SE	3.658	-	0.12	245309
[ME4]2- M=Al, Cr, Mn, Ga, In, Yb, Ni, Cr; E=S, Se, Te	$ZnAl_{1.8}Ga_{0.2}S_4$	*Fd*-3*m*	3D	-	1.508	2.083	0.47	-	SE	3.394	-	0.26	607798
	$ZnAl_2S_4$	*Fd*-3*m*	3D	-	1.507	2.083	0.47	2.60	SE	3.284	-	0.26	609283
	$ZnCr_{1.75}In_{0.25}S_4$	*Fd*-3*m*	3D	-	1.608	2.176	0.51	-	**257**	4.138	1063	0.36	626205
	$ZnCr_2S_4$	*Fd*-3*m*	3D	-	1.615	2.196	0.52	0.04	**270**	3.976	1074	0.09	164169
$[M_3TE_7]^{2-}$ M=La, Ce, Gd; T=Al, Ga; E=S, Se, Te	$ZnLa_3AlS_7$	*P*6$_3$	1D	[001]	1.538	1.916	0.52	2.27	SE	4.496	-	0.23	608324
$[PS_3]^{2-}$	$ZnPS_3$	*C*2/*m*	3D	-	1.548	1.964	0.58	2.10	SE	3.207	-	0.25	79557
[ME4]2- M=Al, Cr, Mn, Ga, In, Yb, Ni, Cr; E=S, Se, Te	**$ZnAlCrS_4$**	*Fd*-3*m*	3D	-	1.604	2.170	0.59	-	**295**	3.630	1071	0.18	606839
$[M_3TE_7]^{2-}$ M=La, Ce, Gd; T=Al, Ga; E=S, Se, Te	$ZnY_6Ge_2S_{14}$	*P*6$_3$	1D	[001]	1.568	2.113	0.72	-	SE	4.132	-	0.34	637813
	$ZnY_6Si_2S_{14}$	*P*6$_3$	1D	[001]	1.578	2.156	0.77	-	SE	3.902	-	0.19	249883
$[ScGaS_4]^{2-}$	$ZnScGaS_4$	*P*-3*m*1	2D	(001)	1.524	1.930	0.90	1.02	SE	3.470	-	0.12	656809
$[TaS_2]^{-}$	$Zn_{0.5}TaS_2$	*P*6$_3$/*mmc*	2D	(001)	1.542	2.065	1.13	-	SE	7.670	-	0.42	651118

$[M_3TE_7]^{2-}$ M=La, Ce, Gd; T=Al, Ga; E=S, Se, Te	$ZnCe_3AlS_7$	$P6_3$	1D	[001]	1.500	1.920	1.17	0.01	SE	4.624	-	0.13	606507
	$ZnGd_3AlS_7$	$P6_3$	1D	[001]	1.500	1.952	1.30	1.38	SE	5.282	-	0.24	607922

*Promising cathode materials and corresponding values of their gravimetric capacities are highlighted in bold.

Table S5. 35 promising ternary and quaternary Al-/S(Se,Te)-containing compounds after the GT analysis sorted in ascending order of the migration barrier energy E_m from BVSE. Electronic band gap energies E_g (if any) were taken from https://materialsproject.org. The theoretical gravimetric capacity C_g was calculated for compounds with electrochemically active transition metals (if the compound does not contain a transition metal, it is indicated as a "SE").

Framework type	Chemical formula	Space Group symmetry		GT			E_m(BVSE), eV	E_g, eV	C_g, mAh/g	ρ, g/cm^3	Cv, mAh/cm^3	*GII*	ICSD-#
			Dimension of migration	Direction of migration	R_{sd}, Å	r_{chan}, Å							
$[BeLa_3S_7]^{3-}$	$AlBeLa_3S_7$	$P6_3$	1D	[001]	1.515	1.931	0.06	2.20	SE	4.202	-	0.45	606164
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}La_6S_{14}$	$P6_3$	1D	[001]	1.524	1.941	0.07	-	SE	4.230	-	0.37	608320
	$Al_{3.3}Dy_6S_{14}$	$P6_3$	1D	[001]	1.503	1.946	0.25	-	SE	5.132	-	0.43	607336
$[CaTe_{10}]^{18-}$	Al_6CaTe_{10}	$P4_132$	3D	-	1.829	2.449	0.33	-	SE	4.518	-	0.19	10046
$[Mg_2Se_5]^{6-}$	$Al_2Mg_2Se_5$	$P\text{-}3m1$	2D	(001)	1.714	2.240	0.33	1.99	SE	3.960	-	0.31	41928
$[MS_4]^{6-}$ M=Mn, Zn	**Al_2MnS_4**	$R3m$	2D	(001)	1.507	1.906	0.34	0.00	**226**	2.752	622	0.35	608511
$[BaS_7]^{3-}$	Al_4BaS_7	$Pmn2_1$	1D	[001]	1.536	1.961	0.37	3.19	SE	2.875	-	0.13	33237
$[MS_4]^{6-}$ M=Mn, Zn	Al_2ZnS_4	$R3m$	2D	(001)	1.531	1.980	0.37	0.00	SE	2.979	-	0.23	609280
$[MgS_4]^{6-}$	Al_2MgS_4	$R\text{-}3m$	2D	(001)	1.577	2.121	0.42	2.02	SE	2.438	-	0.19	107308
$[SnTe_{9.892}]^{18-}$	$Al_{5.9}SnTe_{9.892}$	$P3_121$	3D	-	1.810	2.331	0.45	1.44	SE	4.739	-	0.25	408710
$[(P_2S_6)_3]^{12-}$	$Al_4(P_2S_6)_3$	$C2$	3D	-	1.504	1.901	0.46	2.24	SE	2.472	-	0.34	428186
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}La_6Se_{14}$	$P6_3$	1D	[001]	1.617	2.175	0.59	-	SE	5.756	-	0.24	608326
$[M_3TE_7]^{-}$ M=Sm, Y; E=S, Se, Te	$Al_{0.33}Sm_3SiS_7$	$P6_3$	1D	[001]	1.508	2.150	0.60	-	SE	4.832	-	0.16	249886
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{1.65}Ce_3Se_7$	$P6_3$	1D	[001]	1.609	2.166	0.60	-	SE	5.864	-	0.24	606511
$[M_3TE_7]^{-}$ M=Sm, Y; E=S, Se, Te	$Al_{0.67}Y_6Ge_2S_{14}$	$P6_3$	1D	[001]	1.581	2.139	0.66	-	SE	3.968	-	0.21	425882
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}Pr_6Se_{14}$	$P6_3$	1D	[001]	1.601	2.157	0.69	-	SE	5.970	-	0.27	609111
	$Al_{1.65}Gd_3S_7$	$P6_3$	1D	[001]	1.502	1.933	0.77	-	SE	4.953	-	0.40	607918
	$Al_{3.3}Nd_6Se_{14}$	$P6_3$	1D	[001]	1.651	2.205	0.79	-	SE	6.097	-	0.30	608777
	$Al_{3.3}Sm_6Se_{14}$	$P6_3$	1D	[001]	1.641	2.186	0.83	-	SE	6.306	-	0.36	609318
$[LiP_2S_6]^{3-}$	$AlLiP_2S_6$	$C2/c$	1D	[001]	1.506	1.908	0.89	2.76	SE	2.319	-	0.15	425979
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}Ho_6S_{14}$	$P6_3$	1D	[001]	1.509	1.983	0.98	-	SE	5.290	-	0.43	608216
	$Al_{3.3}Gd_6Se_{14}$	$P6_3$	1D	[001]	1.630	2.167	1.00	-	SE	6.557	-	0.32	607925
	$Al_{3.3}Tb_6Se_{14}$	$P6_3$	1D	[001]	1.628	2.162	1.02	-	SE	6.614	-	0.33	609321
	$Al_{3.3}Dy_6Se_{14}$	$P6_3$	1D	[001]	1.622	2.152	1.08	-	SE	6.758	-	0.36	607337

	$Al_{1.65}Ce_3S_7$	*P*6$_3$	1D	[001]	1.519	1.969	1.17	-	SE	4.338	-	0.17	606503
	$Al_{3.3}Ho_6Se_{14}$	*P*6$_3$	1D	[001]	1.613	2.134	1.20	-	SE	6.914	-	0.42	608217
$[MS_4]^{6-}$ M=Cd, Hg	Al_2HgS_4	*Fd*-3*m*	3D	-	1.508	1.931	1.28	1.70	SE	4.681	-	0.33	608160
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}Pr_6S_{14}$	*P*6$_3$	1D	[001]	1.510	1.939	1.31	-	SE	4.423	-	0.14	609109
$[MS_4]^{6-}$ M=Cd, Hg	Al_2CdS_4	*Fd*-3*m*	3D	-	1.502	1.923	1.36	2.69	SE	3.645	-	0.28	43025
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}Nd_6S_{14}$	*P*6$_3$	1D	[001]	1.504	1.935	1.39	-	SE	4.532	-	0.15	608775
	$Al_{3.3}Sm_6S_{14}$	*P*6$_3$	1D	[001]	1.507	1.954	1.58	-	SE	4.746	-	0.14	609257
	$Al_{3.3}Tb_6S_{14}$	*P*6$_3$	1D	[001]	1.501	1.951	1.83	-	SE	5.039	-	0.16	609262
$[NaP_2S_6]^{3-}$	$AlNaP_2S_6$	*Fdd*2	1D	[1-10]; [110]	1.512	1.939	1.85	2.66	SE	2.200	-	0.18	425980
$[M_3E_7]^{5-}$ M=La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Y; E=S, Se, Te	$Al_{3.3}Y_6S_{14}$	*P*6$_3$	1D	[001]	1.500	1.907	2.42	-	SE	3.807	-	0.32	609267
	$Al_{1.67}Er_3S_7$	*P*6$_3$	1D	[001]	1.503	1.917	2.26	-	SE	5.442	-	0.43	607434

*Promising cathode materials and corresponding values of their gravimetric capacities are highlighted in bold.

Table S6. 40 compounds with a migration energy less than 0.6 eV according to BVSE.

Working Ion	Chemical formula	ICSD-#	*GII*	E_m(dim) (eV)	ΔE_m (eV)	Note
Mg^{2+}	$MgYb_2Se_4$	76053	0.29	0.13	0.10	ΔE_m<0.15 eV
	$MgYb_2S_4$	642803	0.19	0.43	-0.19	ΔE_m<0.15 eV
Ca^{2+}	$Ca_{0.667}K_4Te_3$	71608	0.45	0.38	0.09	ΔE_m<0.15 eV
	$CaIn_2Te_4$	24388	0.20	0.53	-0.22	ΔE_m<0.15 eV
Zn^{2+}	$ZnYb_2Se_4$	652208	0.23	0.17	0.15	Prospective conductor
	$ZnMn_2Se_4$	643609	0.34	0.19	-0.08	ΔE_m<0.15 eV
	$ZnLa_3GaSe_7$	431499	0.29	0.25	0.66	*GII* > 0.26
	$ZnCr_{1.94}In_{0.06}Se_4$	85040	0.19	0.29	0.09	ΔE_m<0.15 eV
	$ZnCr_{1.95}Ni_{0.05}Se_4$	93392	0.46	0.29	-0.26	ΔE_m<0.15 eV
	$Zn_6Cl_2S_5$	419561	1.11	0.29	0.32	*GII* is high. Probably, ill-defined structure
	$ZnCr_{1.6}Ga_{0.4}Se_4$	88795	-	0.30	0.26	*GII* is high. Probably, ill-defined structure
	$ZnCr_2Se_4$	626760	0.05	0.31	0.09	ΔE_m<0.15 eV
	$ZnCr_{1.85}Al_{0.15}Se_4$	157339	0.10	0.33	0.08	ΔE_m<0.15 eV
	$ZnNb_6S_8$	645346	0.81	0.34	-0.32	ΔE_m<0.15 eV
	$Zn_3In_2S_6$	68645	0.23	0.34	-0.10	ΔE_m<0.15 eV
	$ZnMn_2S_4$	643504	0.30	0.36	-0.21	ΔE_m<0.15 eV
	$ZnLa_6Ge_2S_{14}$	636870	0.14	0.43	0.26	Prospective conductor
	$ZnLa_6Si_2S_{14}$	641849	0.13	0.45	0.47	Prospective conductor
	ZnCaOS	245309	0.12	0.46	0.23	Prospective conductor
	$ZnAl_{1.8}Ga_{0.2}S_4$	607798	0.26	0.47	0.30	Prospective conductor
	$ZnAl_2S_4$	609283	0.26	0.47	0.60	Prospective conductor
	$ZnCr_{1.75}In_{0.25}S_4$	626205	0.36	0.51	0.20	*GII* > 0.26 (DFT: $E_m(ZnCr_2S_4)$=2.34 eV)
	$ZnCr_2S_4$	164169	0.09	0.52	-0.09	ΔE_m<0.15 eV
	$ZnLa_3AlS_7$	608324	0.23	0.52	0.71	Prospective conductor
	$ZnPS_3$	79557	0.25	0.58	-0.12	ΔE_m<0.15 eV
	$ZnAlCrS_4$	606839	0.18	0.59	-0.50	ΔE_m<0.15 eV
Al^{3+}	$AlBeLa_3S_7$	606164	0.45	0.06	1.38	*GII* > 0.26
	$Al_{3.3}La_6S_{14}$	608320	0.37	0.07	0.85	*GII* > 0.26
	$Al_{3.3}Dy_6S_{14}$	607336	0.43	0.25	0.57	*GII* > 0.26
	Al_6CaTe_{10}	10046	0.19	0.33	1.11	Prospective conductor
	$Al_2Mg_2Se_5$	41928	0.31	0.33	-0.15	ΔE_m<0.15 eV
	Al_2MnS_4	608511	0.35	0.34	-0.11	ΔE_m<0.15 eV
	Al_4BaS_7	33237	0.13	0.37	0.18	Prospective conductor
	Al_2ZnS_4	609280	0.23	0.37	0.08	ΔE_m<0.15 eV
	Al_2MgS_4	107308	0.19	0.42	-0.20	ΔE_m<0.15 eV
	$Al_{5.9}SnTe_{9.892}$	408710	0.25	0.45	0.64	Prospective conductor
	$Al_4(P_2S_6)_3$	428186	0.34	0.46	-0.06	ΔE_m<0.15 eV
	$Al_{3.3}La_6Se_{14}$	608326	0.24	0.59	0.18	Prospective conductor
	$Al_{0.33}Sm_3SiS_7$	249886	0.16	0.60	0.36	Prospective conductor
	$Al_{1.65}Ce_3Se_7$	606511	0.24	0.60	-0.11	ΔE_m<0.15 eV

*Prospective conductor: fulfillment of all three conditions in section METHODS - BVSE calculations.

**non-fulfillment of at least one of the conditions in section METHODS - BVSE calculations.

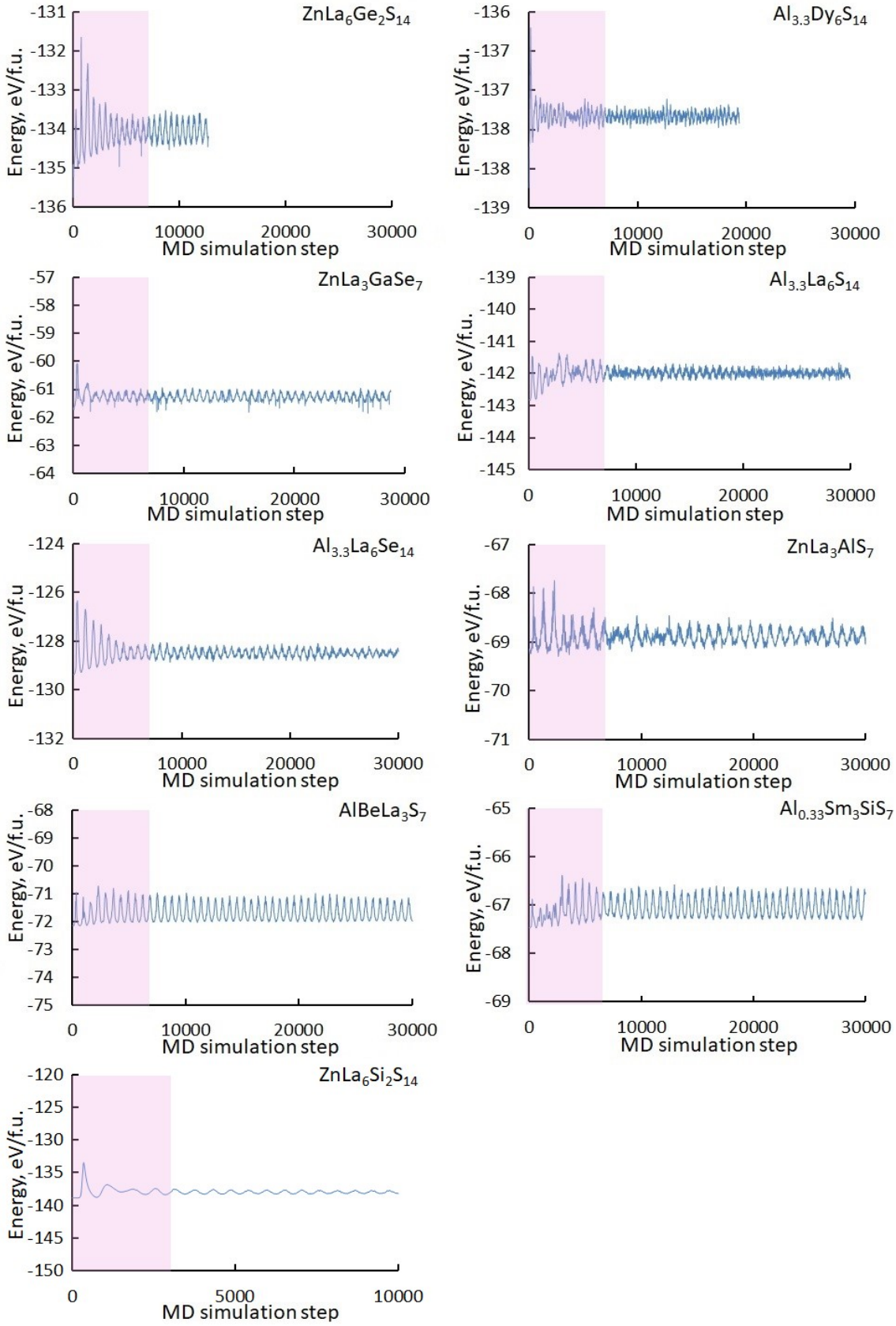

Figure S1. Fluctuations of total energy of the MLn_3TQ_7 structures as a function of the molecular dynamic simulation step (1 step = 1 fs) with 30 ps at 300 K. The first 7 ps of the AIMD simulations are excluded to minimize statistical uncertainty; this area is marked by pink.

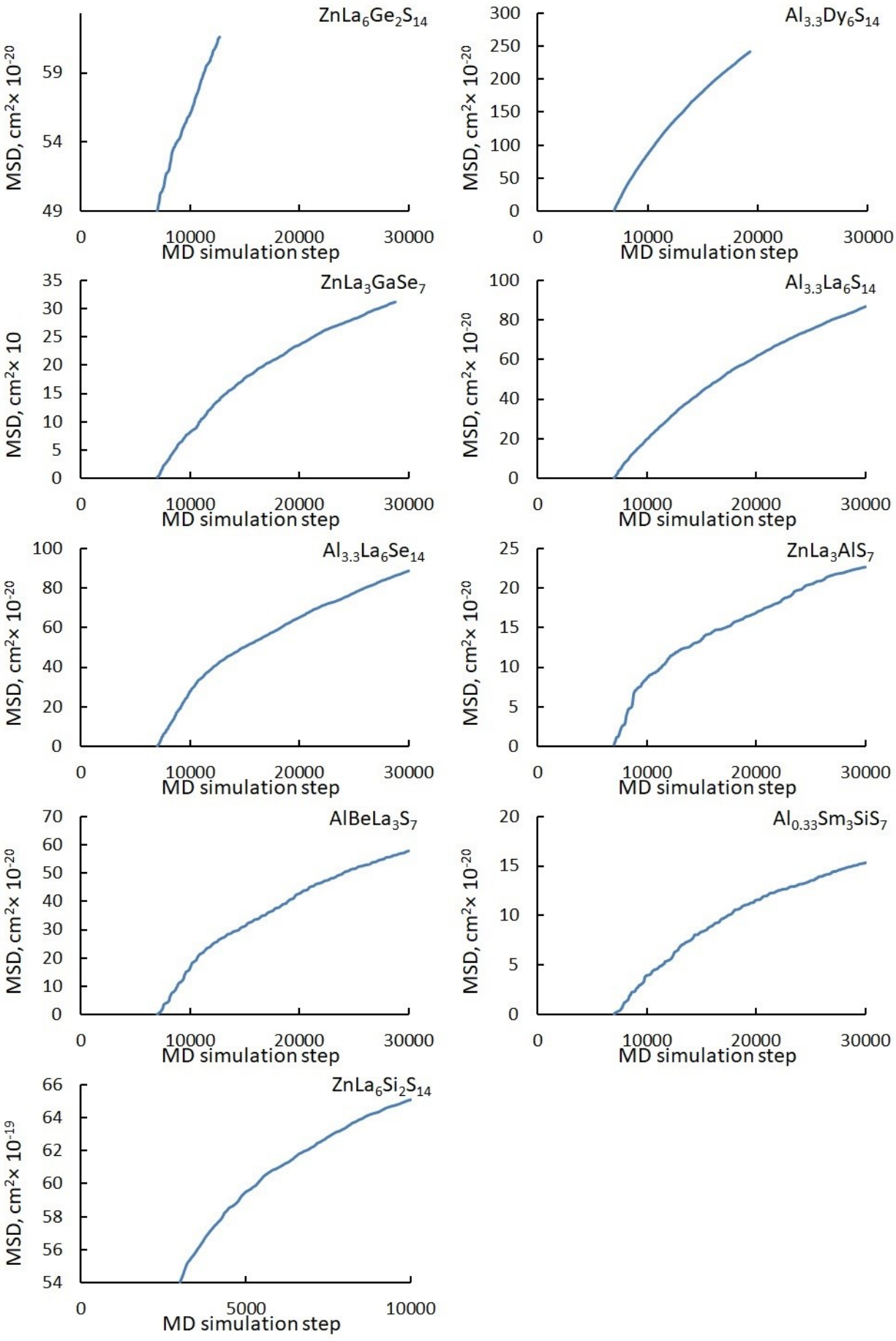

Figure S2. The mean squared displacement (MSD) vs simulation step (1 step = 1 fs) plots for the MLn_3TQ_7 structures from AIMD calculations. The first 7 ps of the AIMD simulations are excluded to minimize statistical uncertainty.