Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Computational investigation of chalcogenide spinel conductors for all-solid-state Mg batteries

Julius Koettgen[a], Christopher J. Bartel[b], and Gerbrand Ceder[a,b,†]

Table S1. Calculated data corresponding with **Figures 2-5**. r_{Ln} = ionic radius of the lanthanoid; V = calculated volume per anion (GGA), E_{mig} = Mg^{2+} migration energy (GGA); $E_{oct} - E_{tet}$ = energy of octahedral state minus energy of tetrahedral state (GGA); spinel, MnY_2S_4, Th_3P_4, Yb_3S_4, olivine = energy above the hull in each of these 5 prototype structures (meta-GGA). "-" appears for structures that were not converged at the meta-GGA level.

compound	r_{Ln} (Å)	V (Å³/anion)	E_{mig} (eV)	$E_{oct} - E_{tet}$ (eV)	spinel (eV/atom)	MnY_2S_4 (eV/atom)	Th_3P_4 (eV/atom)	Yb_3S_4 (eV/atom)	olivine (eV/atom)
$MgLu_2S_4$	0.861	41.510	0.373	0.105	0.006	0.013	0.064	0.062	0.045
$MgLu_2Se_4$	0.861	47.799	0.369	0.079	0.017	0.035	0.085	0.078	0.053
$MgTm_2S_4$	0.880	42.267	0.371	0.125	0.040	0.023	-	0.082	0.060
$MgTm_2Se_4$	0.880	48.605	0.362	0.094	0.021	0.027	0.068	0.073	0.052
$MgEr_2S_4$	0.890	42.728	0.368	0.139	0.048	0.027	0.064	0.087	0.065
$MgEr_2Se_4$	0.890	49.066	0.358	0.100	0.023	0.024	0.061	0.074	0.052
$MgHo_2S_4$	0.901	43.160	0.364	0.151	0.058	0.030	0.064	0.096	0.071
$MgHo_2Se_4$	0.901	49.483	0.355	0.105	0.025	0.020	0.053	0.073	0.051
$MgDy_2S_4$	0.912	43.609	0.361	0.164	0.069	0.034	0.065	0.103	0.077
$MgDy_2Se_4$	0.912	49.968	0.351	0.114	0.058	0.032	0.060	0.089	0.067
$MgTb_2S_4$	0.923	44.140	0.356	0.181	0.080	0.040	0.061	0.112	0.084
$MgTb_2Se_4$	0.923	50.480	0.346	0.122	0.068	0.037	0.059	0.097	0.074
$MgSm_2S_4$	0.958	45.995	0.343	0.237	0.115	0.054	0.067	0.136	0.10
$MgSm_2Se_4$	0.958	52.422	0.334	0.160	0.101	0.051	0.058	0.121	0.097
$MgPm_2S_4$	0.970	46.568	0.339	0.256	-	-	-	-	-
$MgPm_2Se_4$	0.970	53.017	0.330	0.174	0.111	-	-	0.127	0.102
$MgNd_2S_4$	0.983	47.407	0.336	0.283	0.142	0.068	0.071	0.155	0.112
$MgNd_2Se_4$	0.983	53.884	0.323	0.187	0.126	0.063	0.060	0.138	0.110
$MgPr_2S_4$	0.990	48.270	0.335	0.311	0.156	0.074	0.071	0.164	0.117
$MgPr_2Se_4$	0.990	54.801	0.318	0.210	0.139	0.070	0.063	0.148	0.117
$MgLa_2S_4$	1.032	49.504	0.351	0.351	0.178	0.084	0.078	0.172	0.113
$MgLa_2Se_4$	1.032	56.192	0.290	0.240	0.121	0.041	0.032	0.121	0.079