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Supporting Information

High-Performance Sn_2S_3 as a Conversion-Alloying Anode Material for Lithium-Ion Batteries: Insights from First-Principles Calculations

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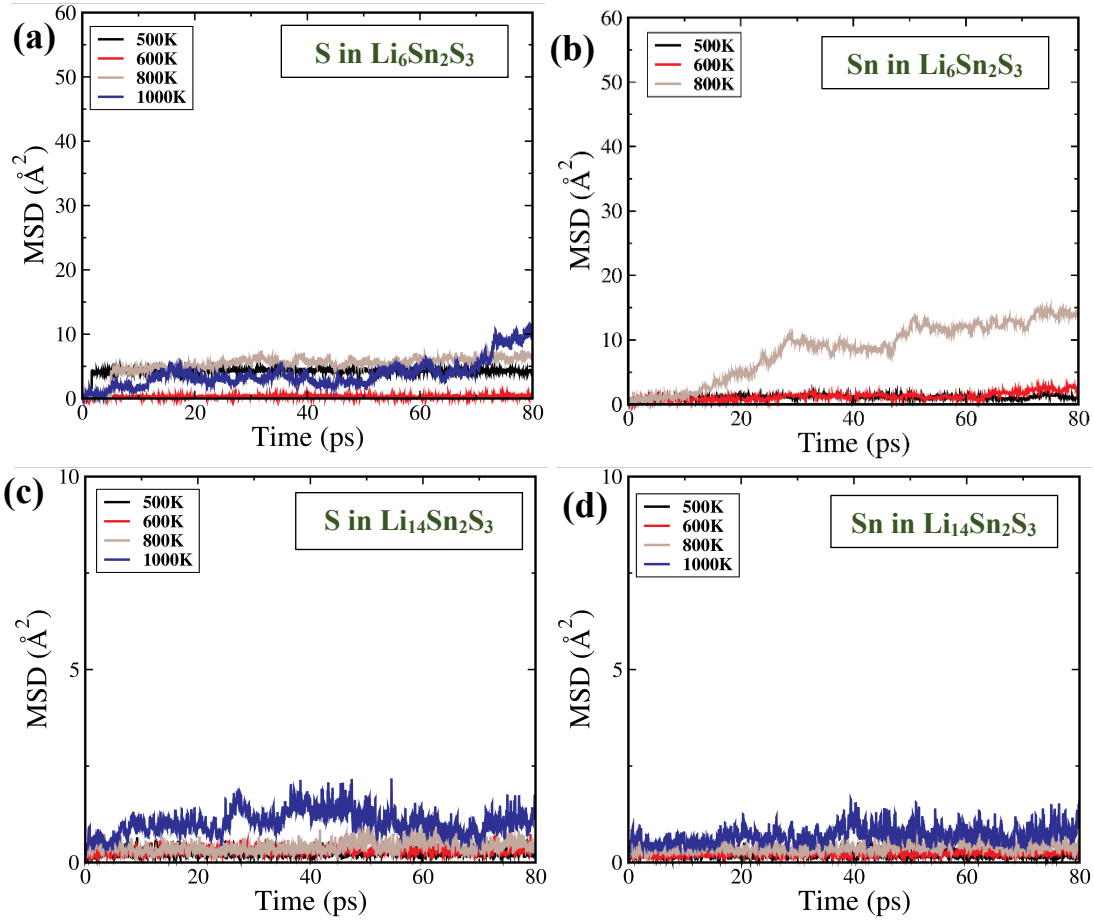

Figure 1: (a) and (b) Mean square displacement (MSD) of S and Sn in $Li_6Sn_2S_3$ 500K, 600K, 800K and 1000K. (c) and (d) Mean square displacement (MSD) of S and Sn in $Li_{14}Sn_2S_3$ at 500K, 600K, 800K and 1000K. The MSD of Sn in $Li_6Sn_2S_3$ at 1000 K is not shown because $Li_6Sn_2S_3$ decomposes into metallic Sn and Li_2S (see Table 4 in main manuscript). Since the melting point of Sn is 505.05 K, Sn melts at this temperature.

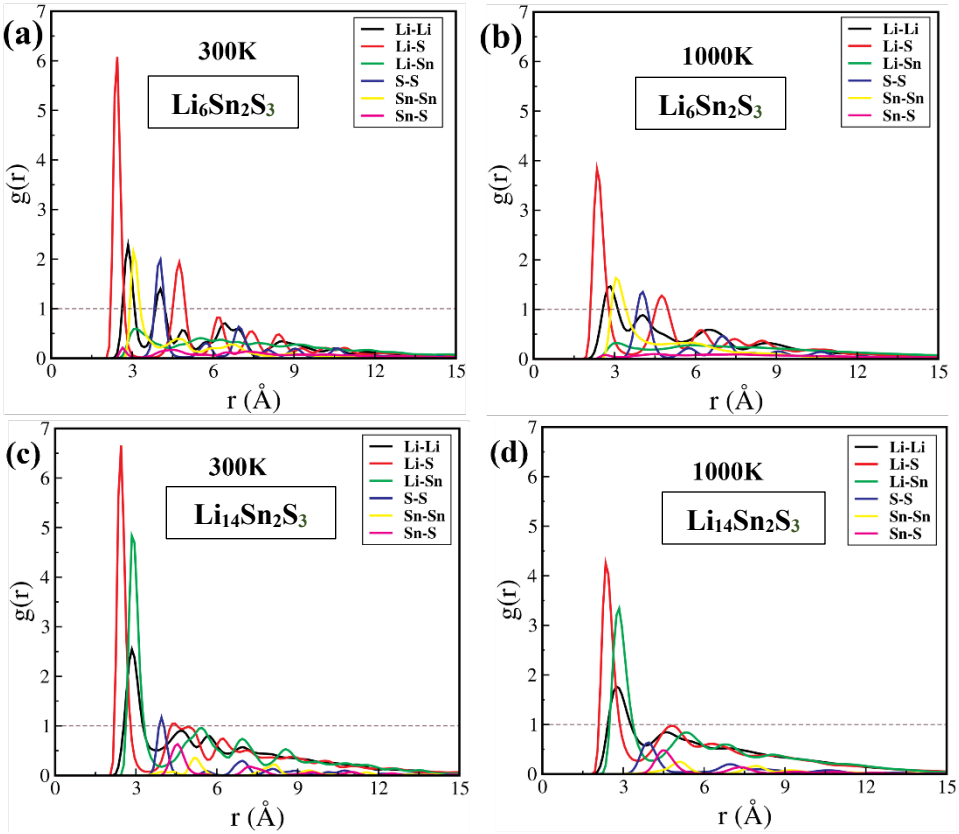

Figure 2: (a) and (b) Radial distribution function (g(r)) in $Li_6Sn_2S_3$ at 300K and 1000K. (c) and (d) Radial distribution function (g(r)) in $Li_{14}Sn_2S_3$ at 300K and 1000K

Table 1: Elastic constants C_{ij} for $Li_xSn_2S_3$ compounds, where all quantities are in units of GPa

	Sn_2S_3	**$Li_{0.25}Sn_2S_3$**	**$Li_{0.5}Sn_2S_3$**	**$Li_2Sn_2S_3$**	**$Li_4Sn_2S_3$**	**$Li_6Sn_2S_3$**	**$Li_8Sn_2S_3$**	**$Li_{14}Sn_2S_3$**
C_{ij}								
C_{11}	31.68	32.48	31.75	65.58	43.49	57.69	57.48	58.22
C_{22}	32.19	42.03	35.67	32.46	52.07	69.74	73.74	59.00
C_{33}	83.20	76.93	75.75	42.61	56.67	52.83	66.42	54.60
C_{44}	14.01	12.91	6.33	13.45	15.54	17.72	29.93	20.71
C_{55}	25.90	21.96	22.17	18.91	16.30	14.56	21.76	20.95
C_{66}	15.13	10.51	6.54	10.93	16.10	21.71	18.62	13.10
C_{12}	16.86	16.47	15.06	16.99	17.76	19.87	20.30	11.74
C_{13}	20.79	18.80	18.47	14.24	18.88	17.37	26.33	10.70
C_{14}		0.06	0.05	-3.11	-0.36	1.36	-0.878	0.47
C_{15}		-0.09	-0.12	1.32	-1.50	4.54	-2.11	-0.29
C_{16}		1.55	3.28	3.04	-0.78	1.24	3.69	-2.89
C_{23}	18.50	19.96	15.84	12.78	14.96	18.34	21.28	14.04
C_{24}		0.21	-0.29	0.69	1.26	0.86	-0.50	-2.35
C_{25}		0.05	-0.05	0.28	-0.11	-0.35	-0.39	-0.95
C_{26}		1.73	-0.52	0.44	0.76	-1.52	-1.68	0.42
C_{34}		0.099	-0.14	5.78	-0.06	3.41	-0.01	0.23
C_{35}		-0.07	-0.003	0.16	2.28	-1.20	-2.68	1.44
C_{36}		1.26	0.36	-0.24	-0.96	0.90	-5.47	2.76
C_{45}		0.59	2.44	-0.19	-1.18	1.58	-0.11	-0.06
C_{46}		-0.008	-0.10	-0.63	-0.38	-0.08	-0.86	1.64
C_{56}		-0.02	0.03	0.16	0.10	-0.84	-0.30	1.45