Supporting Information

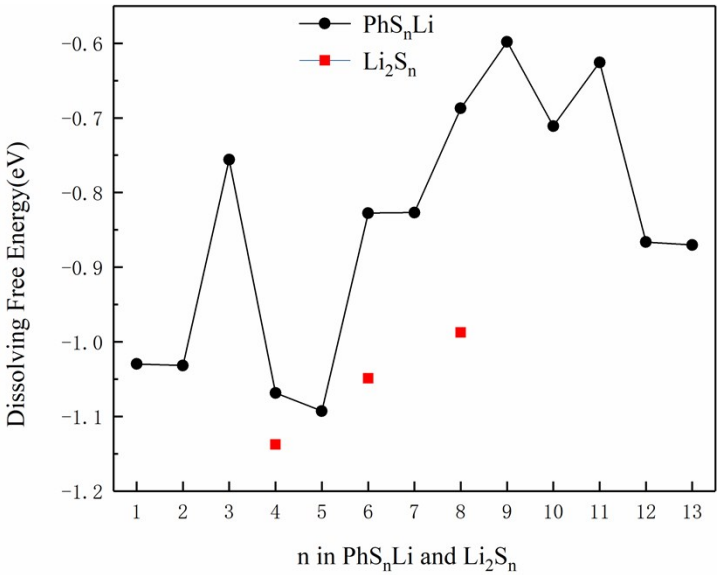

Fig S1 The dissolving free energies of $PhS_nLi(1 \leq n \leq 13)$ and $Li_2S_n(n = 4,6,8)$

Table S1 The discharge reactions, reaction energies and corresponding voltages of PhS_nPh $(1 < n \leq 15)$.

Label	*Category*	*Reactions*	$G_{rec}(eV)$	*Voltage(V)*	*Feasibility*
R_1	PhS_2Ph	$PhS_2Ph + 2Li \rightarrow 2PhSLi$	− 5.07	2.54	√
R_1	PhS_3Ph	$PhS_3Ph + 2Li \rightarrow PhS_2Li + PhSLi$	− 5.11	2.55	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_1	PhS_4Ph	$PhS_4Ph + 2Li \rightarrow 2PhS_2Li$	− 5.13	2.57	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_1	PhS_5Ph	$PhS_5Ph + 2Li \rightarrow PhS_2Li + PhS_3Li$	− 5.05	2.53	√
R_2		$PhS_3Li + 2Li \rightarrow PhSLi + Li_2S_2$	− 5.03	2.52	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	− 3.80	1.90	√
R_1	PhS_6Ph	$PhS_6Ph + 2Li \rightarrow PhS_2Li + PhS_4Li$	− 5.05	2.53	√
R_2		$PhS_4Li + 2Li \rightarrow PhS_2Li + Li_2S_2$	− 4.94	2.47	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	− 3.80	1.90	√
R_1	PhS_7Ph	$PhS_7Ph + 2Li \rightarrow PhS_2Li + PhS_5Li$	− 5.08	2.54	√
R_2		$PhS_5Li + 2Li \rightarrow PhS_3Li + Li_2S_2$	− 5.01	2.51	√
R_2		$PhS_3Li + 2Li \rightarrow PhSLi + Li_2S_2$	− 5.03	2.52	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	− 3.80	1.90	√
R_1	PhS_8Ph	$PhS_8Ph + 2Li \rightarrow PhS_2Li + PhS_6Li$	− 5.29	2.65	√
R_2		$PhS_6Li + 2Li \rightarrow PhS_4Li + Li_2S_2$	− 4.92	2.46	√
R_2		$PhS_4Li + 2Li \rightarrow PhS_2Li + Li_2S_2$	− 4.94	2.47	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	− 3.80	1.90	√
R_1	PhS_9Ph	$PhS_9Ph + 2Li \rightarrow PhS_2Li + PhS_7Li$	− 5.25	2.63	√
R_2		$PhS_7Li + 2Li \rightarrow PhS_5Li + Li_2S_2$	− 4.83	2.42	√
R_2		$PhS_5Li + 2Li \rightarrow PhS_3Li + Li_2S_2$	− 5.01	2.51	√
R_2		$PhS_3Li + 2Li \rightarrow PhSLi + Li_2S_2$	− 5.03	2.52	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	− 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	− 3.80	1.90	√
R_1	$PhS_{10}Ph$	$PhS_{10}Ph + 2Li \rightarrow PhS_2Li + PhS_8Li$	− 5.36	2.68	√

R_2		$PhS_8Li + 2Li \rightarrow PhS_6Li + Li_2S_2$	– 5.04	2.52	√
R_2		$PhS_6Li + 2Li \rightarrow PhS_4Li + Li_2S_2$	– 4.92	2.46	√
R_2		$PhS_4Li + 2Li \rightarrow PhS_2Li + Li_2S_2$	– 4.94	2.47	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	– 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	– 3.80	1.90	√
R_1	$PhS_{11}Ph$	$PhS_{11}Ph + 2Li \rightarrow PhS_2Li + PhS_9Li$	– 4.88	2.44	√
R_2		$PhS_9Li + 2Li \rightarrow PhS_7Li + Li_2S_2$	– 5.49	2.75	√
R_2		$PhS_7Li + 2Li \rightarrow PhS_5Li + Li_2S_2$	– 4.83	2.42	√
R_2		$PhS_5Li + 2Li \rightarrow PhS_3Li + Li_2S_2$	– 5.01	2.51	√
R_2		$PhS_3Li + 2Li \rightarrow PhSLi + Li_2S_2$	– 5.03	2.52	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	– 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	– 3.80	1.90	√
R_1	$PhS_{12}Ph$	$PhS_{12}Ph + 2Li \rightarrow PhS_2Li + PhS_{10}Li$	– 5.31	2.66	√
R_2		$PhS_{10}Li + 2Li \rightarrow PhS_8Li + Li_2S_2$	– 5.07	2.54	√
R_2		$PhS_8Li + 2Li \rightarrow PhS_6Li + Li_2S_2$	– 5.04	2.52	√
R_2		$PhS_6Li + 2Li \rightarrow PhS_4Li + Li_2S_2$	– 4.92	2.46	√
R_2		$PhS_4Li + 2Li \rightarrow PhS_2Li + Li_2S_2$	– 4.94	2.47	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	– 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	– 3.80	1.90	√
R_1	$PhS_{13}Ph$	$PhS_{13}Ph + 2Li \rightarrow PhS_2Li + PhS_{11}Li$	– 4.99	2.50	√
R_2		$PhS_{11}Li + 2Li \rightarrow PhS_9Li + Li_2S_2$	– 4.83	2.42	√
R_2		$PhS_9Li + 2Li \rightarrow PhS_7Li + Li_2S_2$	– 5.49	2.75	√
R_2		$PhS_7Li + 2Li \rightarrow PhS_5Li + Li_2S_2$	– 4.83	2.42	√
R_2		$PhS_5Li + 2Li \rightarrow PhS_3Li + Li_2S_2$	– 5.01	2.51	√
R_2		$PhS_3Li + 2Li \rightarrow PhSLi + Li_2S_2$	– 5.03	2.52	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	– 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	– 3.80	1.90	√
R_1	$PhS_{14}Ph$	$PhS_{14}Ph + 2Li \rightarrow PhS_2Li + PhS_{12}Li$	– 5.21	2.61	√
R_2		$PhS_{12}Li + 2Li \rightarrow PhS_{10}Li + Li_2S_2$	– 5.03	2.52	√
R_2		$PhS_{10}Li + 2Li \rightarrow PhS_8Li + Li_2S_2$	– 5.07	2.54	√
R_2		$PhS_8Li + 2Li \rightarrow PhS_6Li + Li_2S_2$	– 5.04	2.52	√
R_2		$PhS_6Li + 2Li \rightarrow PhS_4Li + Li_2S_2$	– 4.92	2.46	√
R_2		$PhS_4Li + 2Li \rightarrow PhS_2Li + Li_2S_2$	– 4.94	2.47	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	– 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	– 3.80	1.90	√
R_1	$PhS_{15}Ph$	$PhS_{15}Ph + 2Li \rightarrow PhS_2Li + PhS_{13}Li$	– 5.23	2.62	√
R_2		$PhS_{13}Li + 2Li \rightarrow PhS_{11}Li + Li_2S_2$	– 4.79	2.40	√
R_2		$PhS_{11}Li + 2Li \rightarrow PhS_9Li + Li_2S_2$	– 4.83	2.42	√
R_2		$PhS_9Li + 2Li \rightarrow PhS_7Li + Li_2S_2$	– 5.49	2.75	√
R_2		$PhS_7Li + 2Li \rightarrow PhS_5Li + Li_2S_2$	– 4.83	2.42	√
R_2		$PhS_5Li + 2Li \rightarrow PhS_3Li + Li_2S_2$	– 5.01	2.51	√
R_2		$PhS_3Li + 2Li \rightarrow PhSLi + Li_2S_2$	– 5.03	2.52	√
R_3		$PhS_2Li + 2Li \rightarrow PhSLi + Li_2S$	– 4.36	2.18	√
R_3		$Li_2S_2 + 2Li \rightarrow 2Li_2S$	– 3.80	1.90	√