

**TABLE 1.** The adsorption energies ( $E_{\text{ads}}$ ), shortest distances ( $d_{\text{X-AMs}}$ , X = Li or S), charge transfer ( $\Delta Q_{\text{AMs}}$ ) of polysulfides on As, Sb and Bi monolayers.

		S <sub>8</sub>	Li <sub>2</sub> S <sub>8</sub>	Li <sub>2</sub> S <sub>6</sub>	Li <sub>2</sub> S <sub>4</sub>	Li <sub>2</sub> S <sub>2</sub>	Li <sub>2</sub> S
As	$E_{\text{ads}}$ (eV)	1.03	2.32	2.09	2.16	2.55	3.60
	$d_{\text{X-As}}$ (Å)	3.30	2.71	2.72	2.73	2.76	2.26
	$\Delta Q_{\text{As}}$ (e)	0.04	0.11	0.08	0.08	-0.03	-0.31
	$\Delta Q_{\text{Li}}$ (e)	—	-0.19	-0.18	-0.24	-0.20	0.01
	$\Delta Q_{\text{S}}$ (e)	-0.04	0.08	0.10	0.16	0.23	0.30
Sb	$E_{\text{ads}}$ (eV)	1.19	1.82	1.60	1.65	1.88	2.70
	$d_{\text{X-Sb}}$ (Å)	3.50	2.88	2.92	2.89	2.90	2.60
	$\Delta Q_{\text{Sb}}$ (e)	0.11	0.16	0.10	0.13	0.07	-0.10
	$\Delta Q_{\text{Li}}$ (e)	—	-0.12	-0.15	-0.25	-0.24	-0.08
	$\Delta Q_{\text{S}}$ (e)	-0.11	-0.04	0.05	0.12	0.17	0.18
Bi	$E_{\text{ads}}$ (eV)	1.47	2.15	1.76	1.78	1.99	2.67
	$d_{\text{X-Bi}}$ (Å)	3.46	2.95	2.98	2.97	2.97	2.74
	$\Delta Q_{\text{Bi}}$ (e)	0.21	0.46	0.17	0.17	0.11	0.02
	$\Delta Q_{\text{Li}}$ (e)	—	-0.17	-0.15	-0.25	-0.24	-0.13
	$\Delta Q_{\text{S}}$ (e)	-0.21	-0.29	-0.02	0.08	0.13	0.11

**TABLE 2.** Diffusion energy barriers ( $E_{\text{armchair}}/E_{\text{zigzag}}$ ) of Li<sub>2</sub>S<sub>n</sub> (n=4, 6) along armchair and zigzag directions of three anchoring materials.

	Li <sub>2</sub> S <sub>n</sub>	$E_{\text{armchair}}$ (eV)	$E_{\text{zigzag}}$ (eV)
As	Li <sub>2</sub> S <sub>4</sub>	0.73	0.66
	Li <sub>2</sub> S <sub>6</sub>	1.02	0.49
Sb	Li <sub>2</sub> S <sub>4</sub>	1.22	0.79
	Li <sub>2</sub> S <sub>6</sub>	1.10	0.63
Bi	Li <sub>2</sub> S <sub>4</sub>	2.42	0.80
	Li <sub>2</sub> S <sub>6</sub>	1.71	0.79