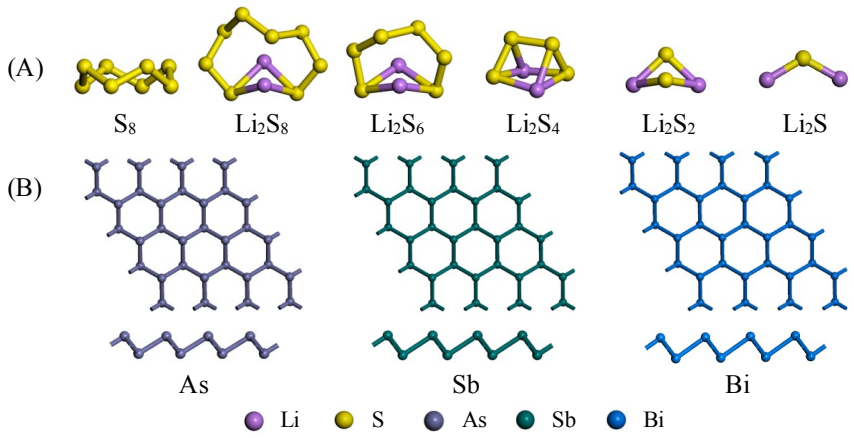


FIGURE 1 (A) Optimized structures of polysulfides at various lithiation stages. (B) Optimized structures of As, Sb and Bi monolayers, both top view (up) and side view (down) are shown.

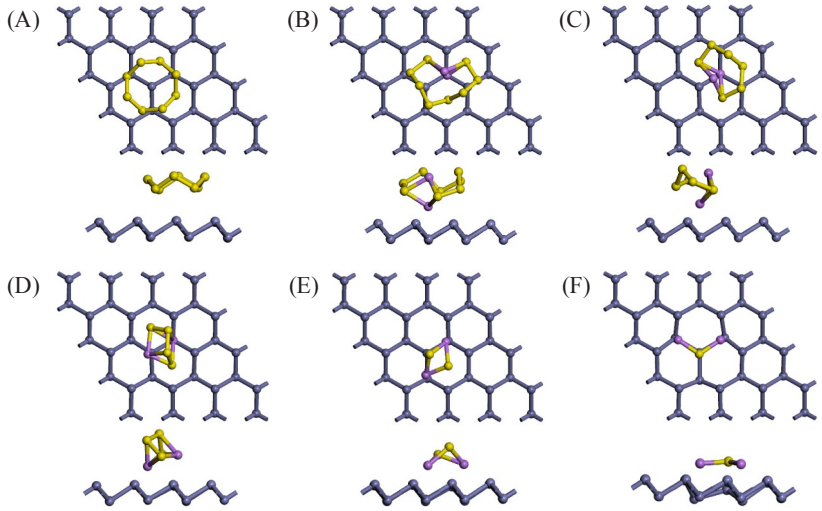


FIGURE 2 The most stable adsorption configurations of (A) S_8 and (B)~(F) Li_2S_n (n = 8, 6, 4, 2, 1) on As monolayer, both top view (up) and side view (down) are shown.

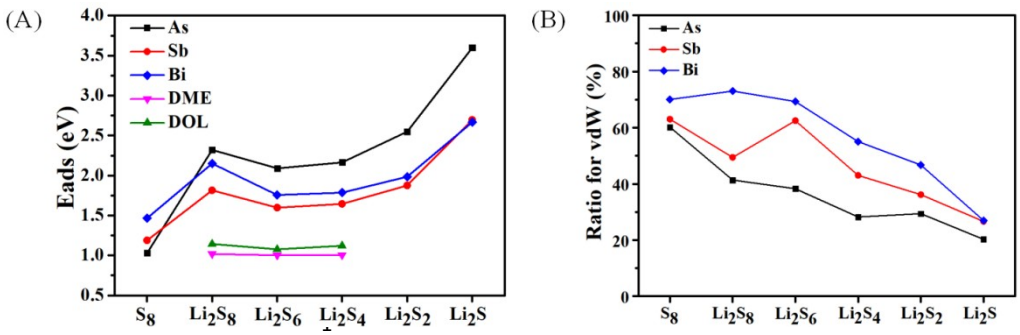


FIGURE 3 (A) Adsorption energies of polysulfides on As, Sb and Bi monolayers. Interaction between polysulfides and DME or DOL were listed for comparison. (B) Ratio for vdW interaction of As, Sb and Bi monolayers at different lithiation stages.

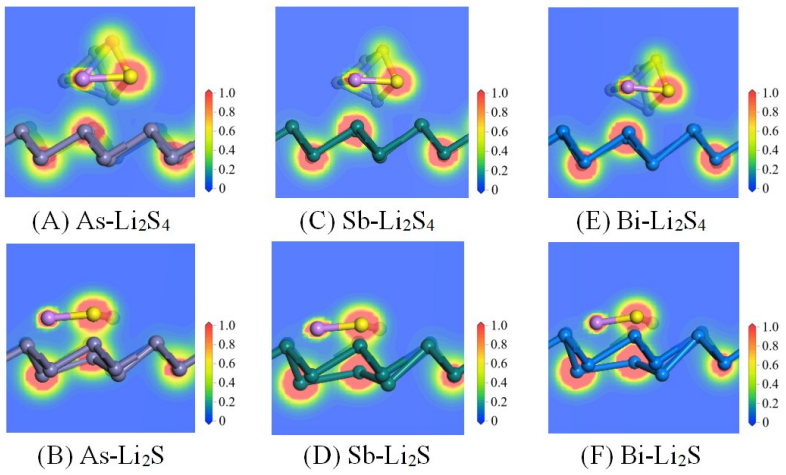


FIGURE 4 Electron density of Li_2S_4 and Li_2S on three anchoring materials.

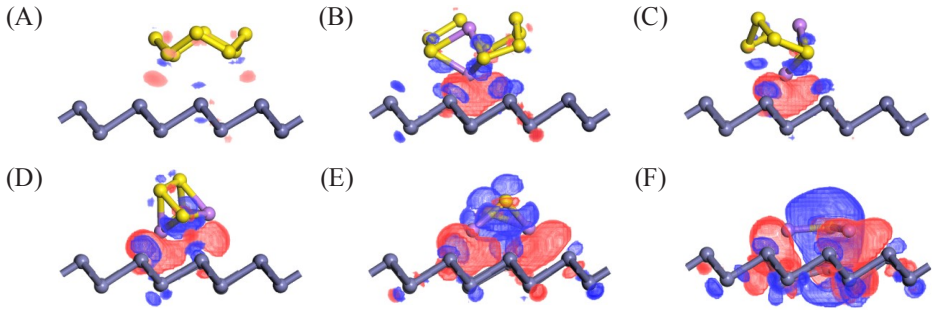


FIGURE 5 Electron density difference of (A) S_8 and (B)~(F) Li_2S_n (n = 8, 6, 4, 2, 1) on As monolayer.

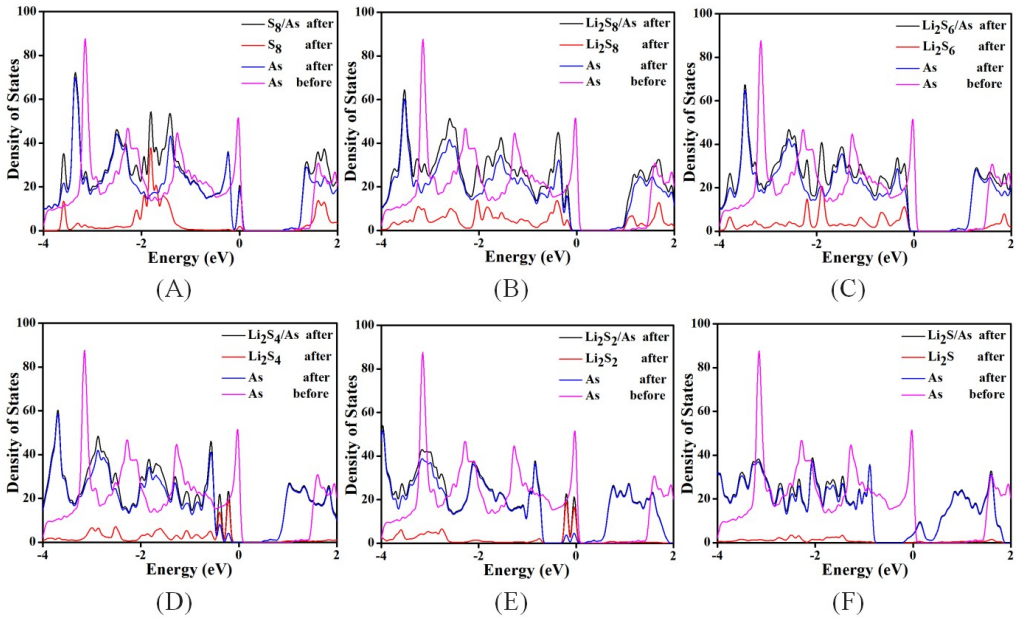
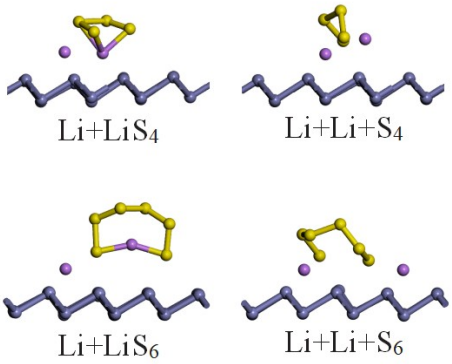


FIGURE 6 DOS of (A) S_8 and (B)~(F) Li_2S_n (n = 8, 6, 4, 2, 1) adsorbed on As monolayer. For comparison, the DOS of isolated As monolayer before adsorption are

presented.

(A)



(B)

	△E1 (eV)	△E2 (eV)
Li_2S_4-As	-0.84	-0.19
Li_2S_4-Sb	-0.22	-0.72
Li_2S_4-Bi	-0.41	-0.76

	△E1 (eV)	△E2 (eV)
Li_2S_6-As	-0.99	-0.80
Li_2S_6-Sb	-0.17	-1.26
Li_2S_6-Bi	-0.38	-0.39

FIGURE 7 (A) Atomic configurations for Li + LiS_n and Li + Li + S_n (n = 4, 6) adsorbed on As monolayer. (B) Energy differences between intact and decomposed configurations adsorbed on different anchoring materials.