

Supplementary Information (SI)

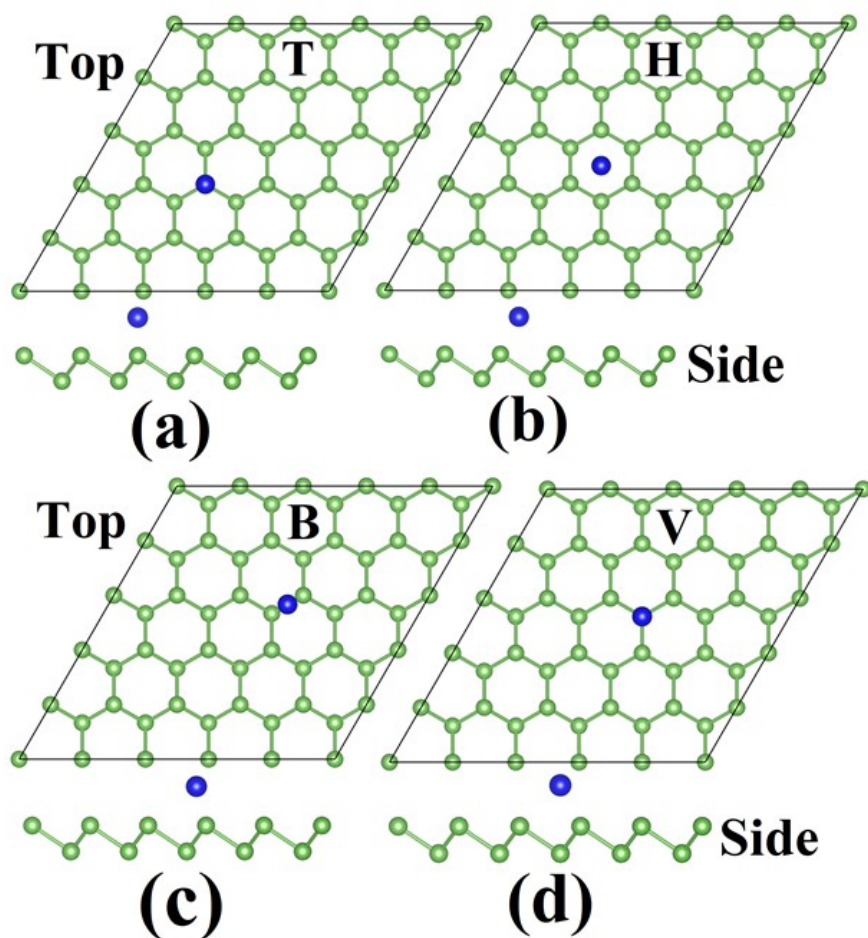


Figure S1: Initial structures of Al-adsorbed arsenene in (a) top (T), (b) hollow (H), (c) bridge (B) and (d) valley (V) site.

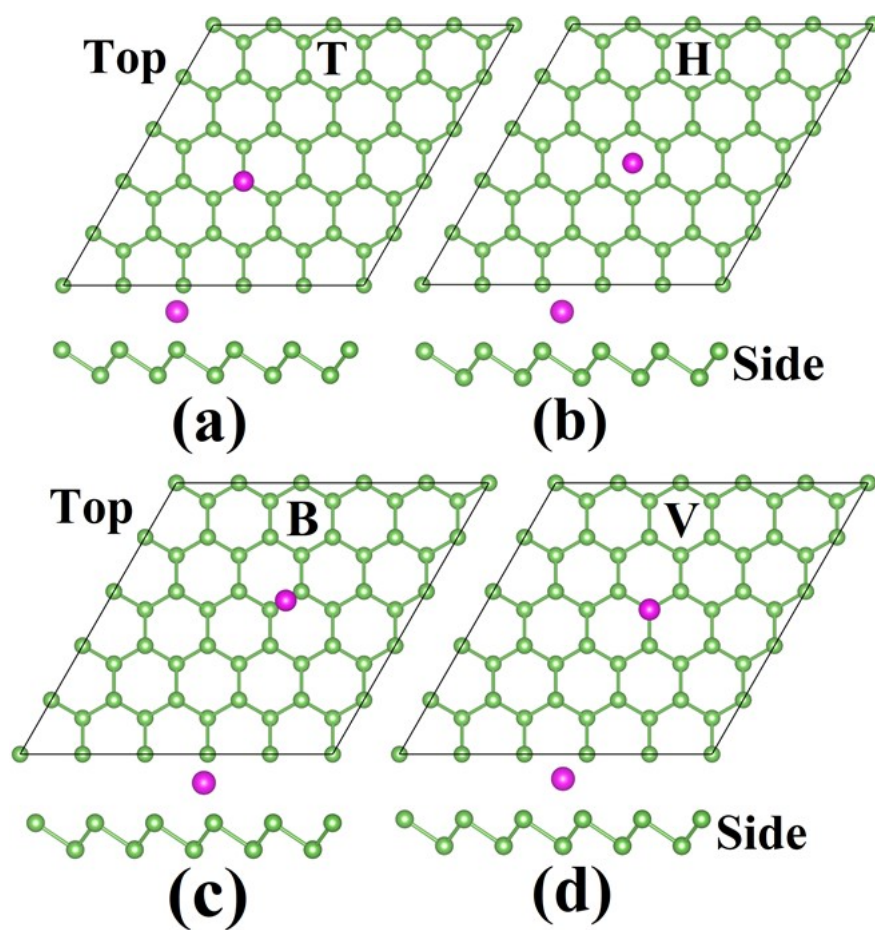


Figure S2: Initial structures of Sn-adsorbed arsenene in (a) top (T), (b) hollow (H), (c) bridge (B) and (d) valley (V) site.

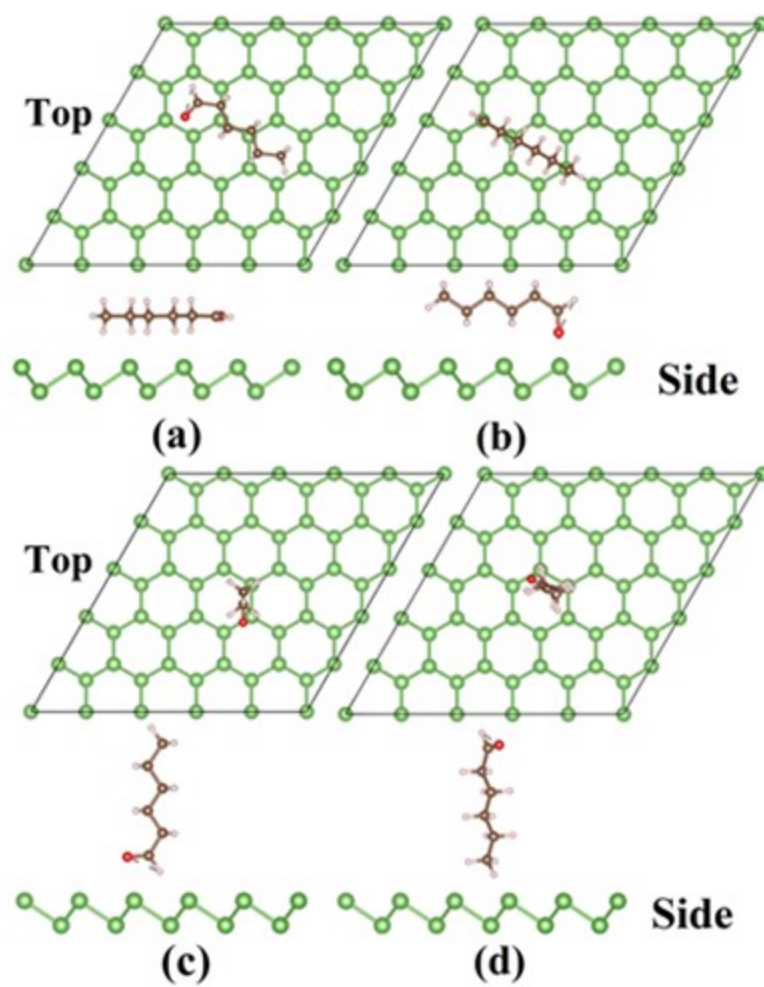


Figure S3: Initial configuration of Hexanal molecule on pristine arsenene (a) horizontal-a (b) horizontal-b (c) vertical-1 (d) vertical-2.

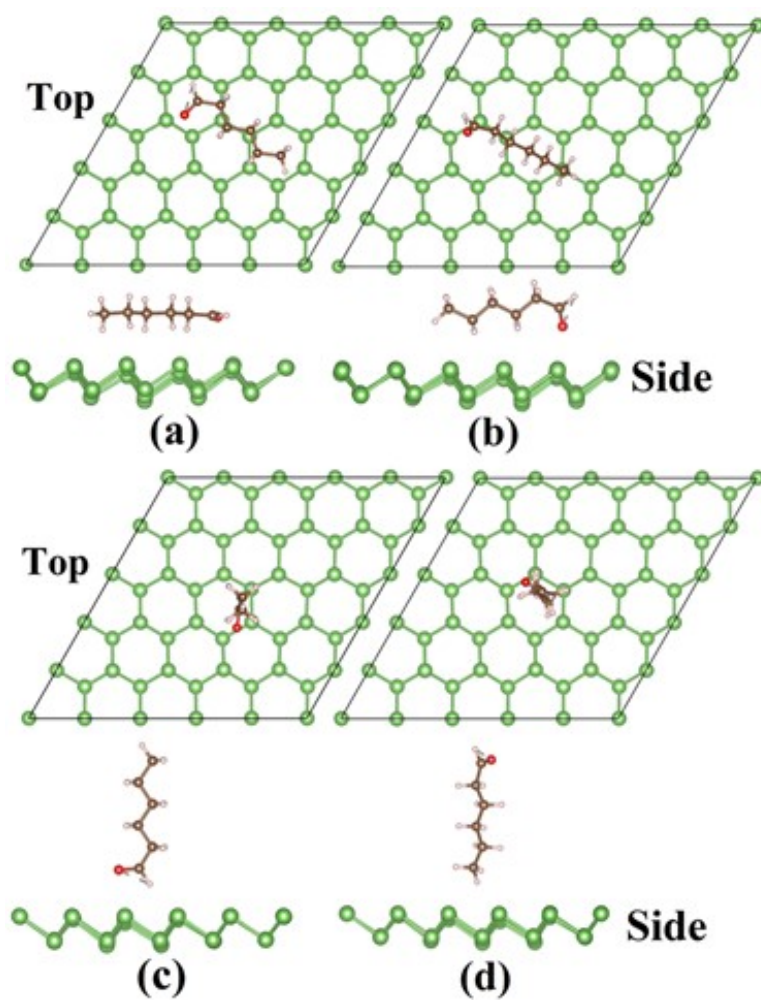


Figure S4: Final configuration of Hexanal molecule on pristine arsenene (a) horizontal-a (b) horizontal-b (c) vertical-1 (d) vertical-2.

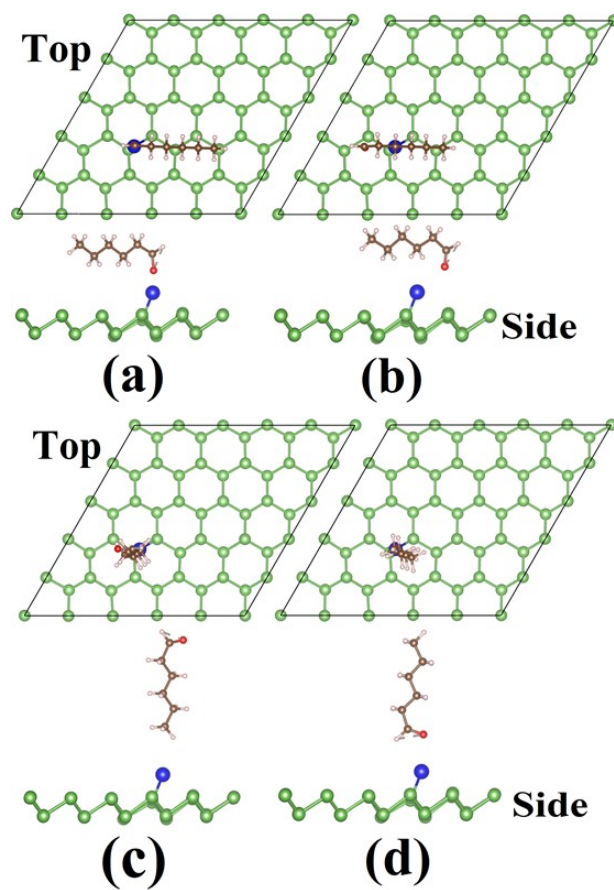


Figure S5: Initial configuration of Hexanal molecule on Al-adsorbed arsenene (a) horizontal-a (b) horizontal-b (c) vertical-1 (d) vertical-2.

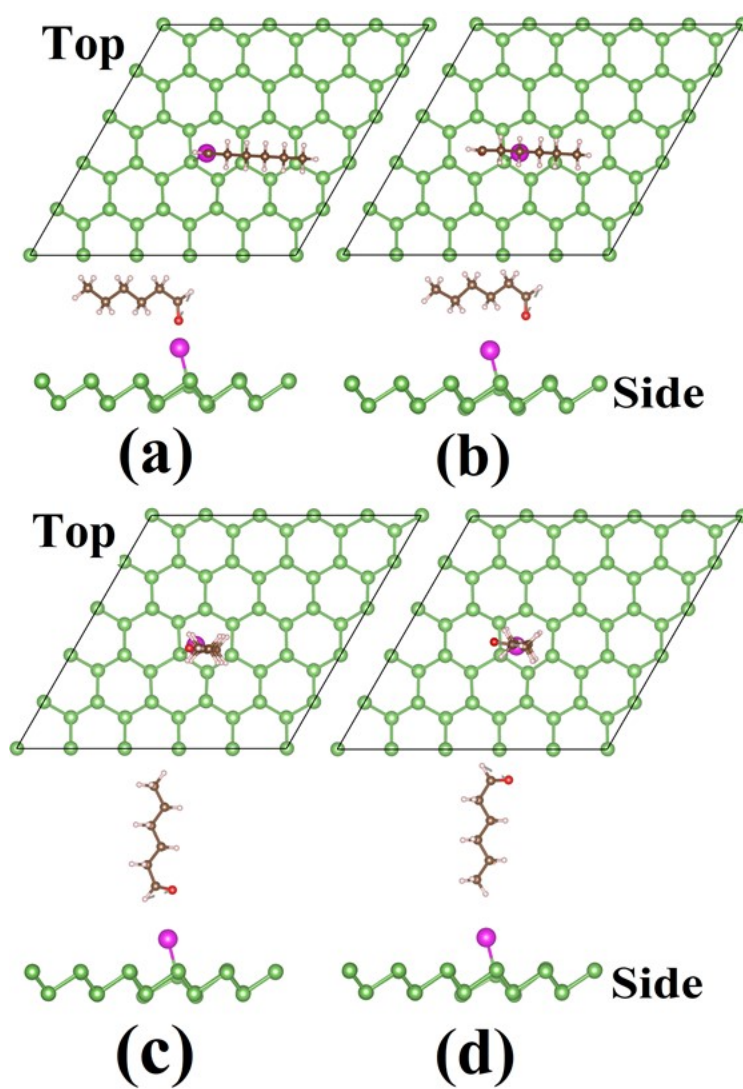


Figure S6: Initial configuration of Hexanal molecule on Sn-adsorbed arsenene (a) horizontal-a (b) horizontal-b (c) vertical-1 (d) vertical-2.

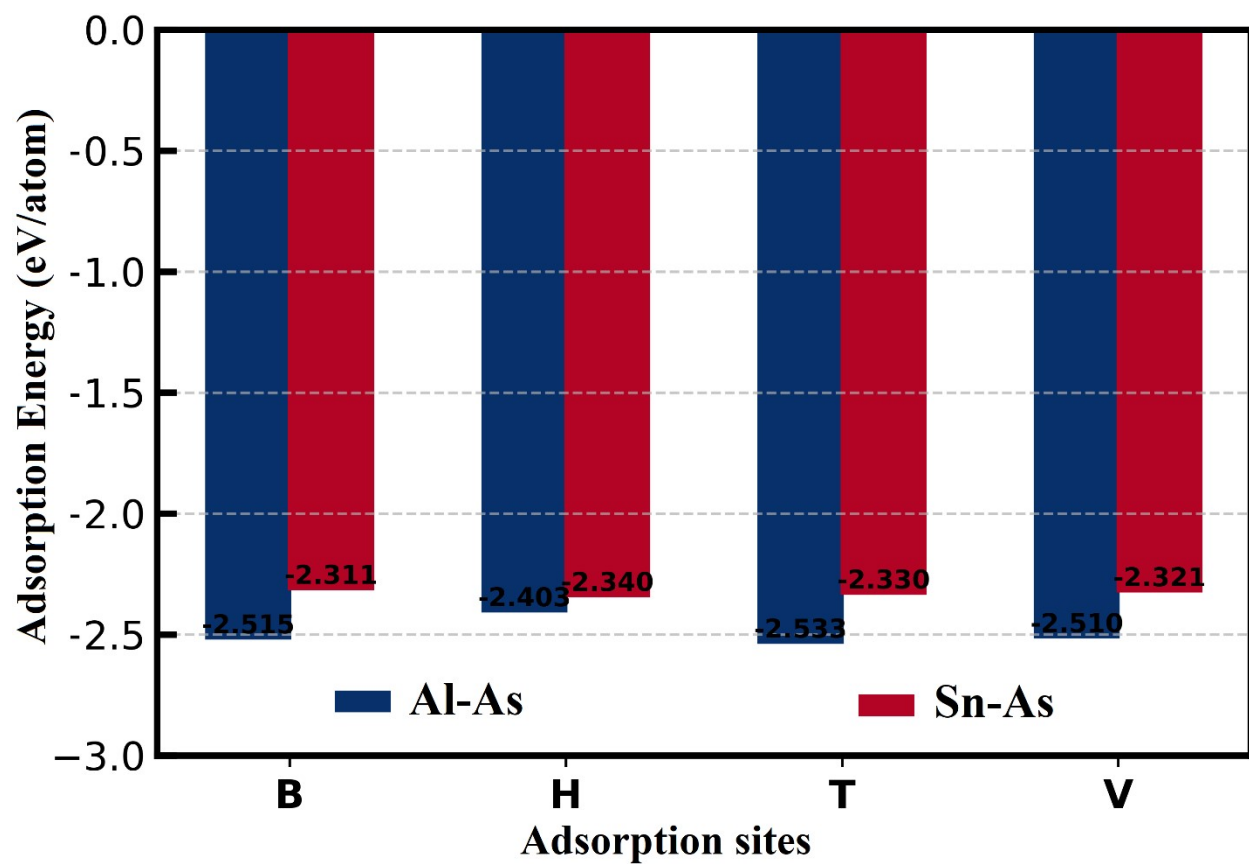


Figure S7: Adsorption energy for single Al/Sn-atom adsorption on bridge (B), hollow (H), top (T), and valley (V) sites of arsenene.