

Metallic CoSb and Janus Co₂AsSb monolayers as a Promising Anode Materials for Metal-Ion Batteries

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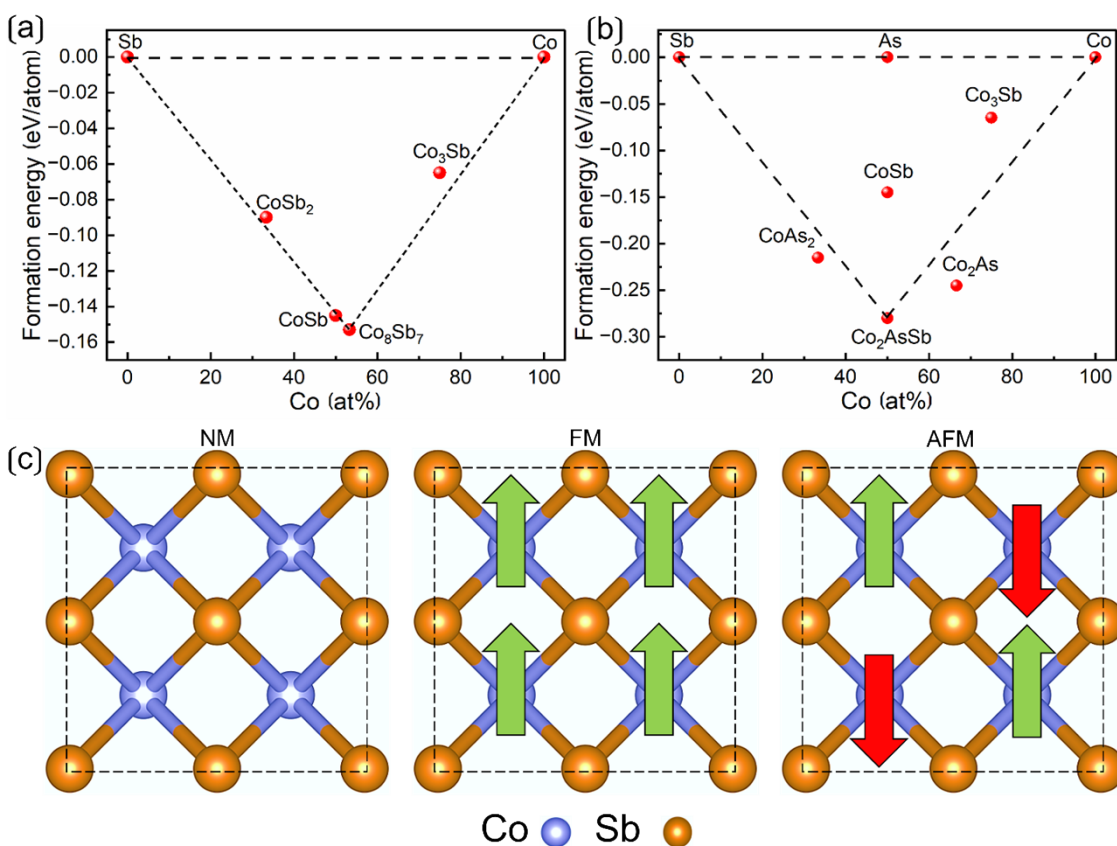


Fig. S1 Formation energy-based convex hull plots, considering different Co compositions for: (a) CoSb and (b) Janus Co₂AsSb monolayers. (c) Three commonly considered magnetic configurations for energetically stable CoSb: (nonmagnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM)).

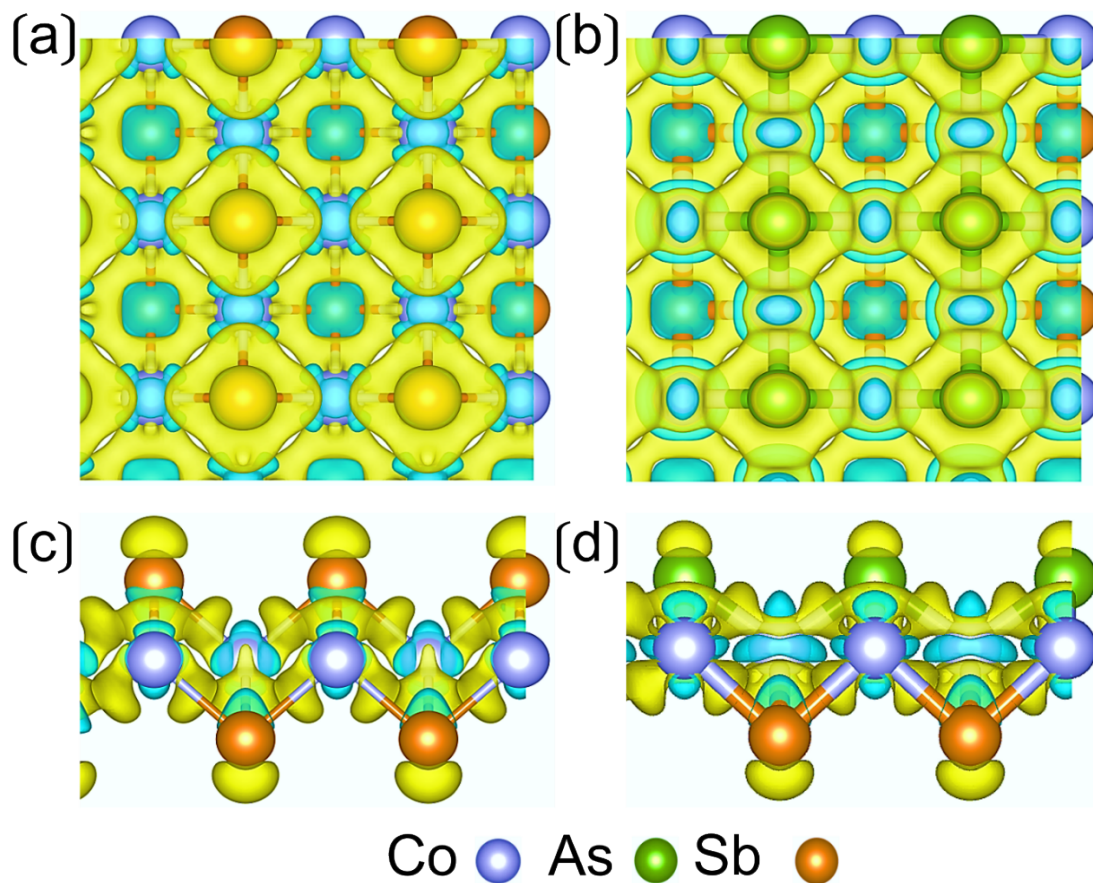


Fig. S2 Charge density difference in CoSb and Janus Co₂AsSb monolayers. Panels (a, c) show top and side views of the CoSb monolayer, while panels (b, d) depict top and side views of the Janus Co₂AsSb monolayer. The iso-surface is set at $0.005 \text{ e}\text{\AA}^3$, with charge accumulation and depletion areas represented in yellow and cyan, respectively.

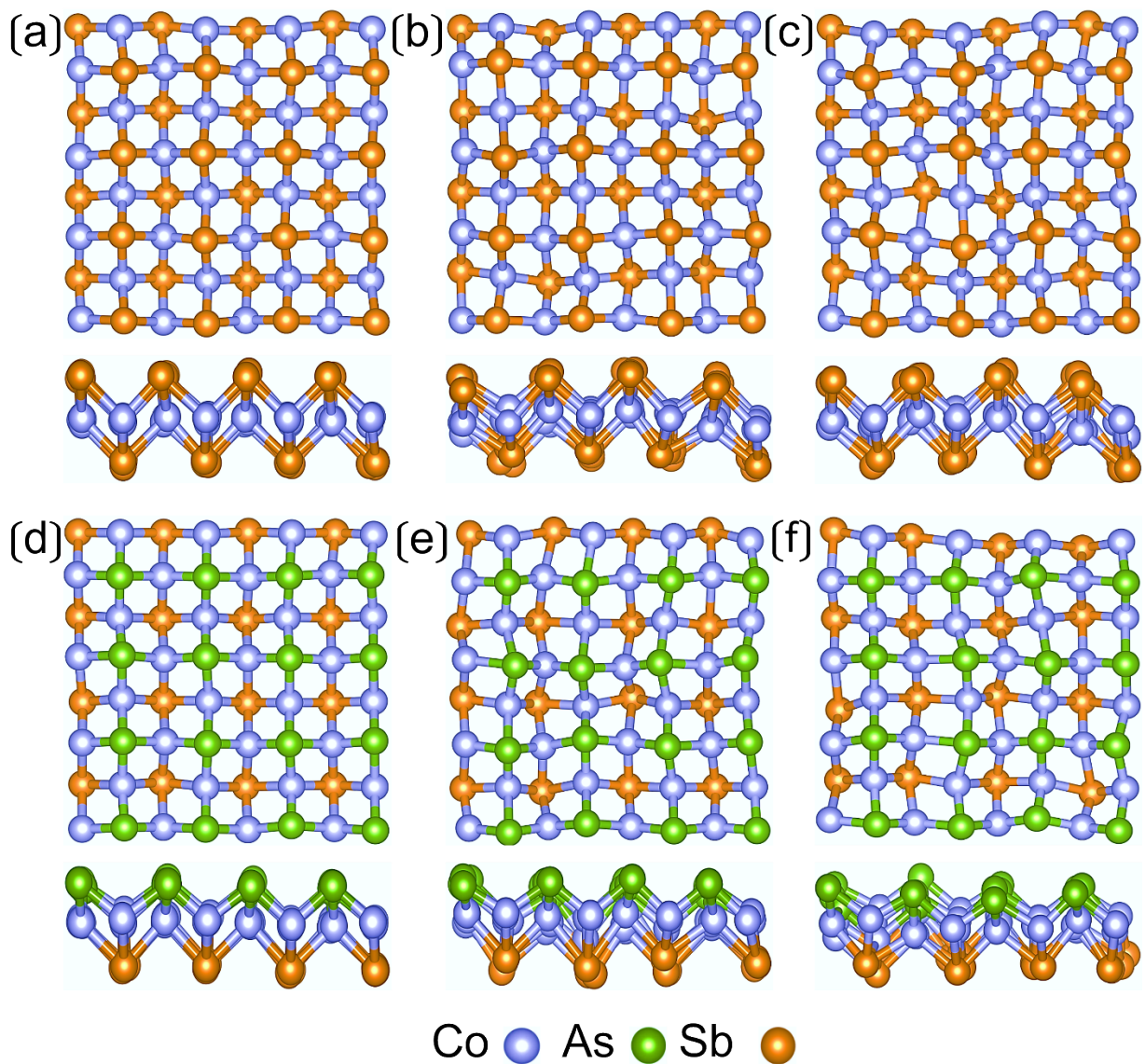


Fig. S3 Atomic structures of CoSb and Janus Co_2AsSb monolayers at the end of 5ps AIMD simulations. This figure displays the top and side views of the CoSb monolayer ($4 \times 4 \times 1$ supercell) at temperatures of (a) 300 K, (b) 600 K, and (c) 900K, along with Co_2AsSb monolayer ($4 \times 4 \times 1$ supercell) at (d) 300 K, (e) 600 K, and (f) 900K, respectively.

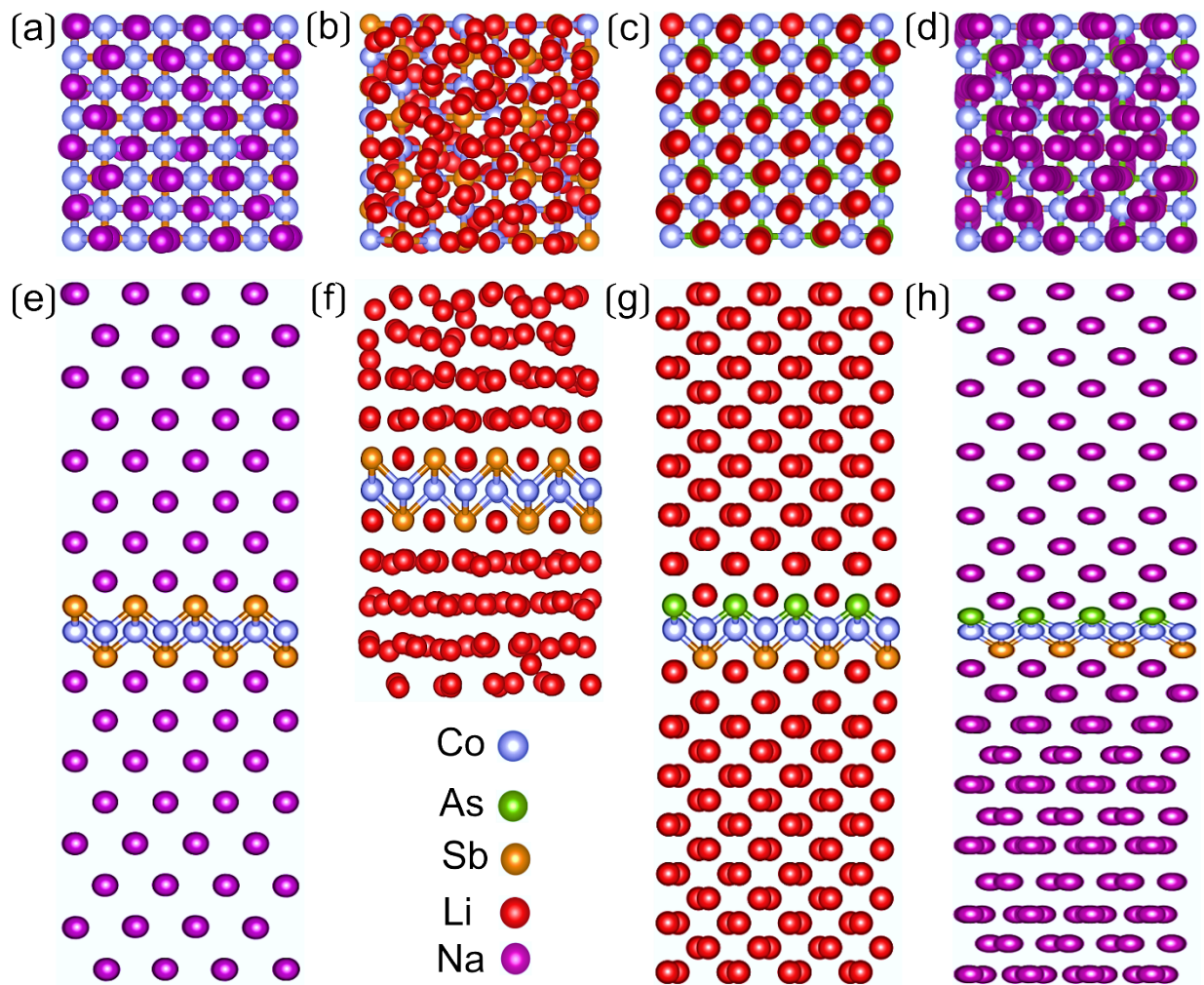


Fig. S4 Top and side views of fully sodiated and fully lithiated monolayers. The figure presents top views of (a) sodiated CoSb, (b) lithiated CoSb, (c) lithiated Janus Co₂AsSb, (d) sodiated Janus Co₂AsSb, followed by side views of (e) sodiated CoSb, (f) lithiated CoSb, (g) lithiated Janus Co₂AsSb, and (h) sodiated Janus Co₂AsSb monolayers.

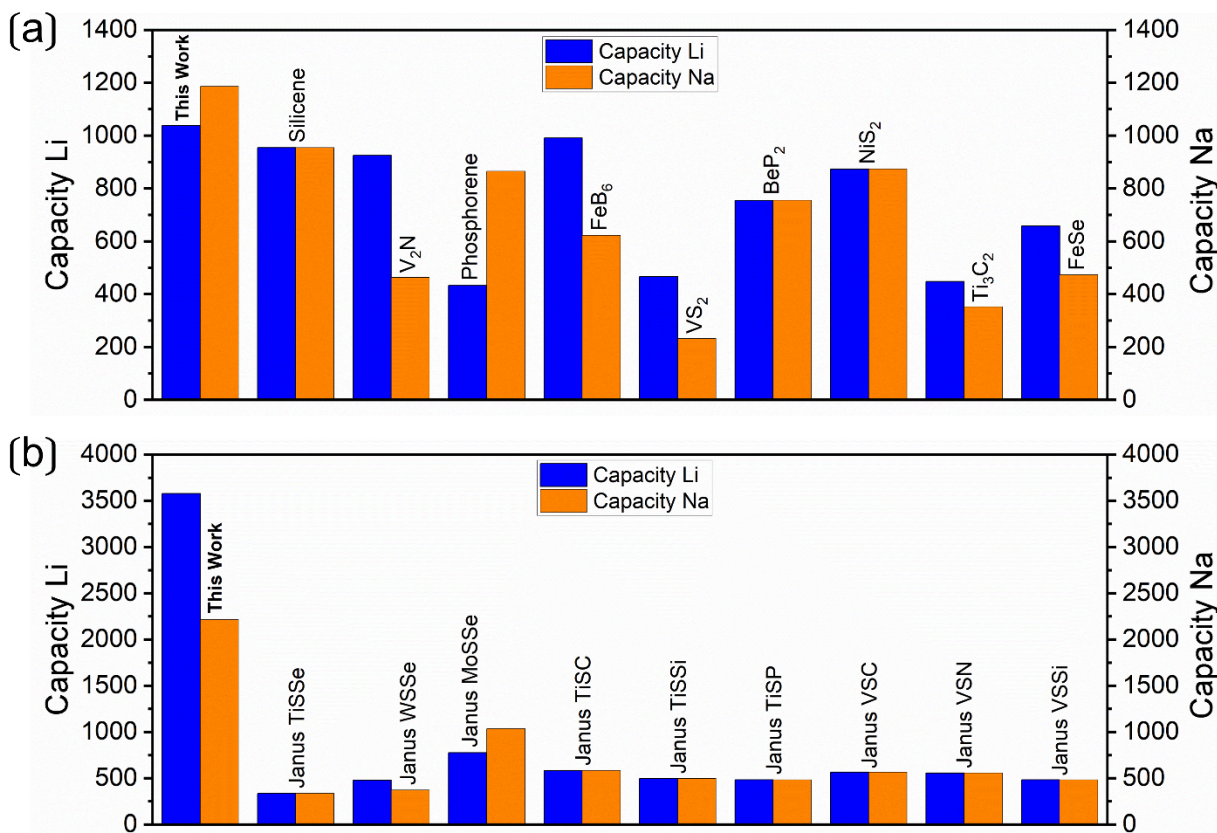


Fig. S5 (a) Comparative analysis of the theoretical specific capacity of Li/Na for various materials including Silicene ^{1,2}, V_2N ³, Phosphorene ^{4,5}, FeB_6 ⁶, VS_2 ^{7,8}, BeP_2 ⁹, NiS_2 ¹⁰, Ti_3C_2 ¹¹, $FeSe$ ¹², and this work (CoSb monolayer). (b) Comparative analysis of the theoretical specific capacity of Li/Na for Janus structures, including $TiSSe$ ¹³, $WSSe$ ¹⁴, $MoSSe$ ^{15,16}, $TiSC$ ¹⁷, $TiSSi$ ¹⁷, $TiSP$ ¹⁷, VSC ¹⁷, VSN ¹⁷, $VSSi$ ¹⁷, and this work (Janus Co_2AsSb monolayer).

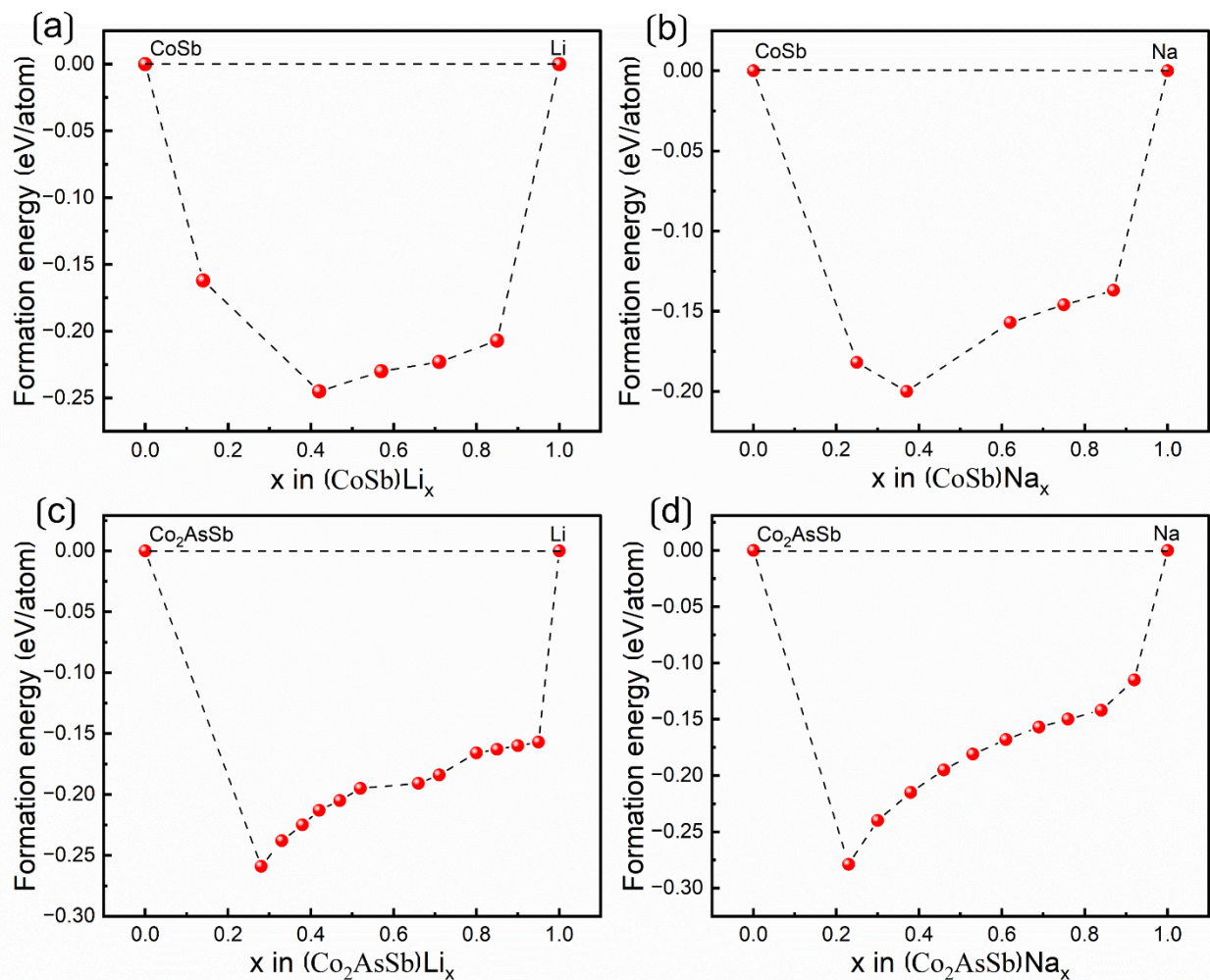


Fig. S6 Formation energy-based convex hull plots for: (a) Li-intercalated CoSb, (b) Na-intercalated CoSb, (c) Li-intercalated Janus Co_2AsSb and (d) Na-intercalated Janus Co_2AsSb .

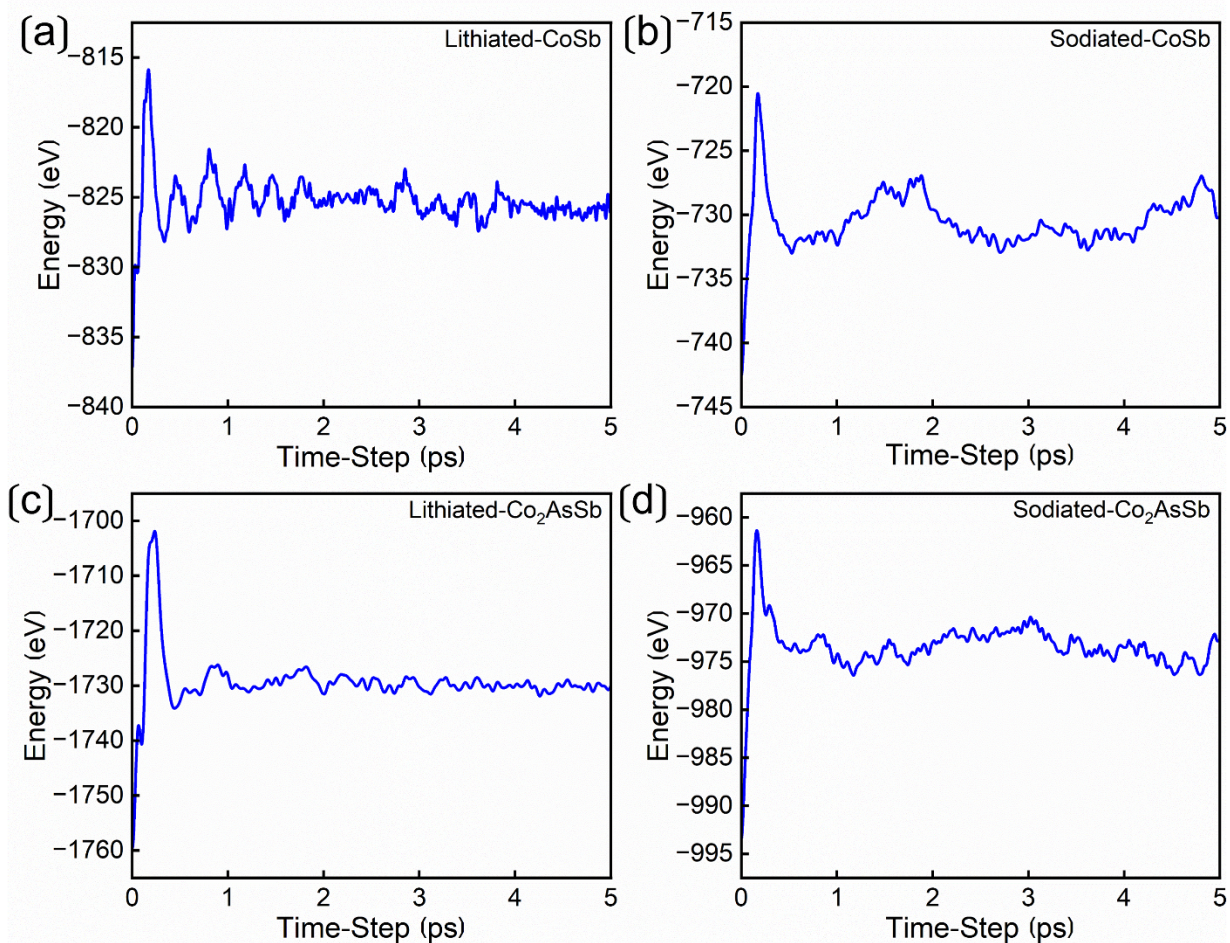


Fig. S7 Evolution of total energy in AIMD simulations at 300K over a 5.0 ps timescale for: (a) fully lithiated CoSb, (b) fully sodiated CoSb, (c) fully lithiated Janus Co₂AsSb and (d) fully sodiated Janus Co₂AsSb monolayers. These results indicate that both monolayered systems are thermodynamically stable.

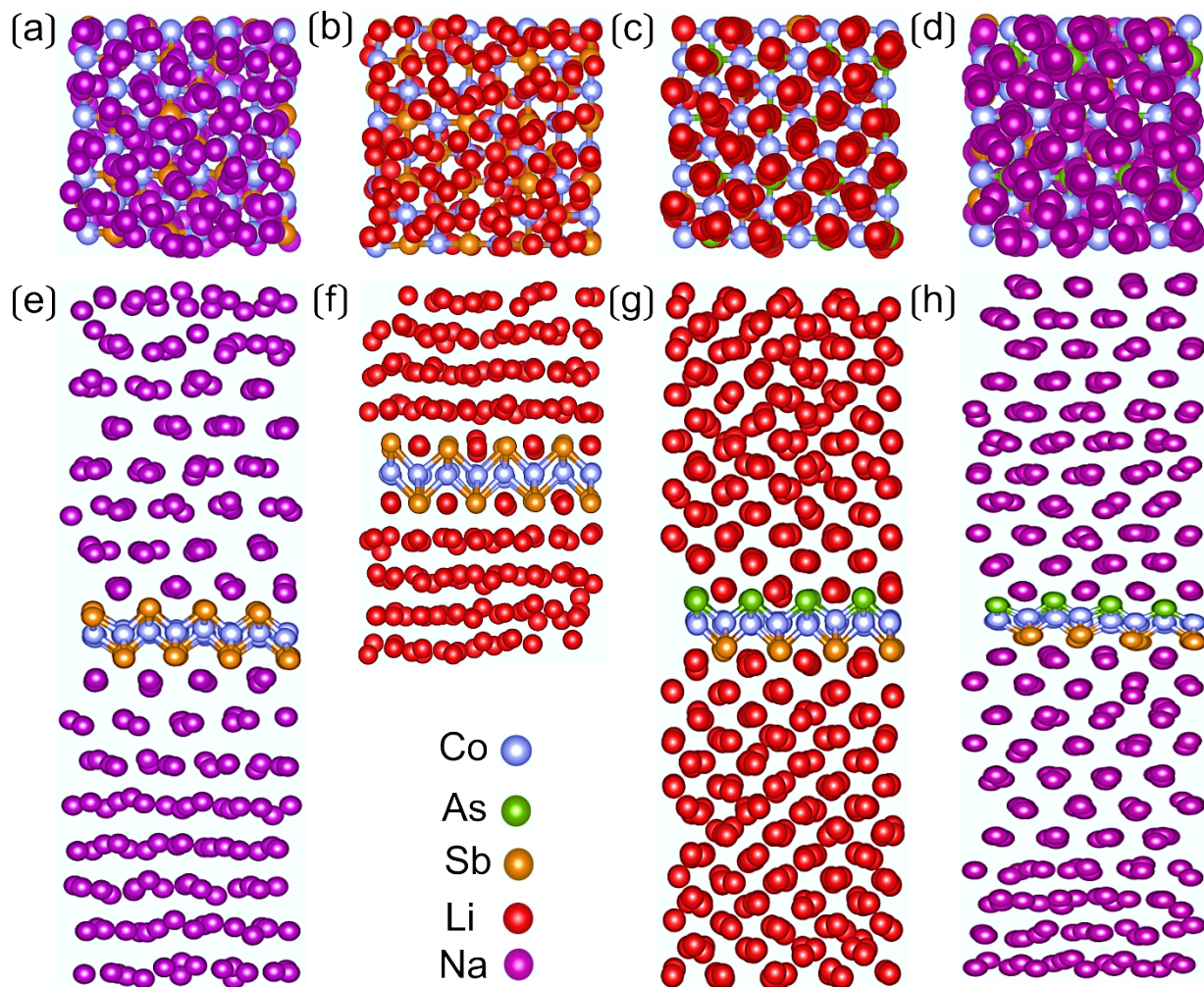


Fig. S8. Geometric configurations of fully lithiated and fully sodiated CoSb and Janus Co₂AsSb monolayers observed during AIMD simulations at 300K over a timescale of 5 ps. The Figure also presents top views of (a) sodiated CoSb, (b) lithiated CoSb, (c) lithiated Janus Co₂AsSb, (d) sodiated Janus Co₂AsSb, followed by side views of (e) sodiated CoSb, (f) lithiated CoSb, (g) lithiated Janus Co₂AsSb, and (h) sodiated Janus Co₂AsSb monolayers.

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