

Theoretical Prediction of Janus Co₂AsSb Monolayer as An Anode Material for Metal-Ion Batteries

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The field of condensed matter physics is rapidly advancing in the domain of two-dimensional (2D) materials. The transition from initial discovery to potential device applications in these enigmatic 2D systems is critically dependent on the pursuit of innovative modifications. Transition metal dichalcogenides have been extensively explored for their Janus modifications.¹ However, to date, the spotlighted 2D systems (tetragonal structure-based, specifically CoSb) have not been reported from a Janus perspective. By employing density functional theory (DFT) computations, we have investigated the electrochemical performance of two-dimensional (2D) CoSb and their Janus Co₂AsSb monolayers for potential applications as anode materials in alkali metal-ion batteries. Our investigation delved into the electronic structure, thermal stability, adsorption, diffusion, and storage behavior of lithium (Li) and sodium (Na) atoms within CoSb and their Janus Co₂AsSb. Our results unveiled that the CoSb and Janus Co₂AsSb monolayers manifest intrinsic metallic properties, which guarantee superior electrical conductivity.

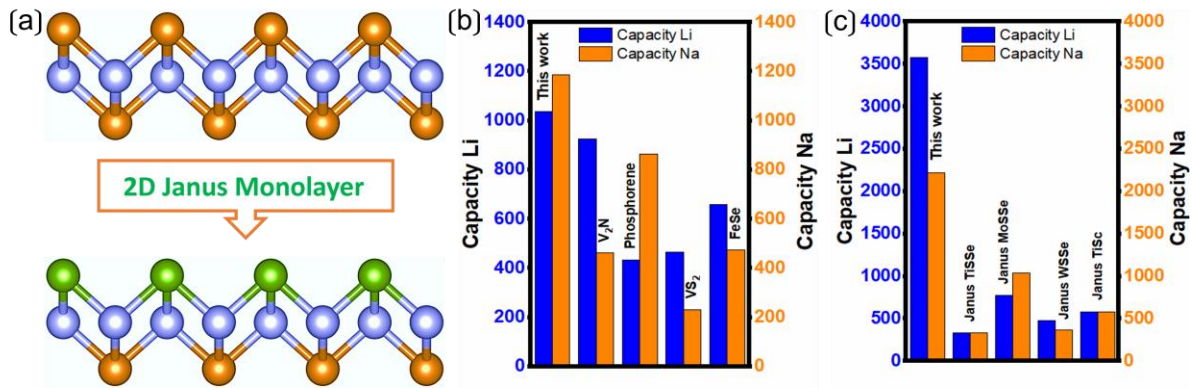


Figure 1. (a) Side views of the CoSb and Janus Co₂AsSb monolayers. (b) Comparative analysis of the theoretical specific capacity of Li/Na for various materials including V₂N², Phosphorene^{3,4}, VS₂^{5,6}, FeSe⁷, and this work (CoSb monolayer). (c) Comparative analysis of the theoretical specific capacity of Li/Na for various Janus materials including TiSSe⁸, MoSSe^{9,10}, WSSe¹¹, TiSC¹², and this work (Janus Co₂AsSb monolayer).

Structural symmetry-breaking plays a pivotal role in fine-tuning the properties of nano-layered materials. In this attempt, we deliver the earnestly-sought solution and proposed: a Janus structure of CoSb, achieved by replacing the antimony in the upper layer with iso-valent arsenic as shown in Fig. 1(a). This modification results in Janus Co₂AsSb, which maintains iso-valency with CoSb, thus preserving similar chemical characteristics. Based on van der Waals (vdW) corrected first-principles approaches, we demonstrate that Janus Co₂AsSb exhibits stability at an elevated temperature of 1200 K, surpassing the stability of CoSb, which is maintained only up to 900 K. This aspect is highly desirable for the growth and eventual mass production of Co₂AsSb.

Furthermore, CoSb and Co₂AsSb can be directly utilized as platforms for novel electrochemical energy storage devices, offering advantages such as relatively high binding strength and ultrafast diffusivity. Our research concludes that CoSb exhibits moderate Li/Na electrochemical storage capabilities, as previously reported for other materials. However, we observed superior electrochemical characteristics in the Janus

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Co₂AsSb, with storage capacities of 3578.69 mA h g⁻¹ for Li and 2215.38 mA h g⁻¹ for Na (see Fig.1(b) & 1(c), representing a significant leap forward in this field. All these encouraging results suggest that 2D CoSb and their Janus Co₂AsSb monolayers hold promise as advanced anode materials for metal ion batteries.

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BIOGRAPHY



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