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Energetic and electronic properties of K-Sb and Na-Sb binary crystals from high-throughput ab initio calculations

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Alkali-based photocathode materials have come into the limelight as novel semiconducting materials for electron sources. However, the study of the fundamental properties of alkali antimonide photocathodes is currently hindered by the limited purity of the samples and the complexity of the growth process.
First-principles studies can effectively complement experiments to gain insight into the stability and the electronic structure of these compounds. In this work, we investigate K-Sb and Na-Sb binary crystals taking input structures available from computational databases. Adopting automatized routines for density functional theory as implemented in the in-house developed library aim2dat [1], we evaluate the energetic stability of the scrutinized materials by generating a convex hull of stable crystals as a function of the relative ratio between the involved species. The absolute minimum of the convex hull for the Na-Sb compounds corresponds to the 3:1 stoichiometry extensively predicted and characterized experimentally. On the other hand, among the K-Sb compounds, the convex hull forms a plateau of stable structures between 1:1 and 3:1 ratios. We analyze the electronic properties of the stable crystals focusing on the correlation between band-gaps and material composition. The analysis of the electronic properties of representative stable compounds for both sets of structures highlights similarities, especially for the known cubic phases Na3Sb and K3Sb, but also remarkable differences. K-based semiconductors span a smaller range of band gap values up to 1.3 eV, while Na-containing crystals have larger band gaps up to 2.5 eV. For the Na-Sb binaries, there is a clear trend relating the size of the band gap with the relative Na content: indirect low-band-gap semiconductors are found among Na-poor phases while large, direct semiconductors appear with 3:1 Na-Sb ratio. In both sets of compounds, metallic phases appear.
Our results [2] provide useful indications to predict and characterize binary phases forming during the growth of multi-alkali antimonide photocathodes. Additionally, the analysis of the electronic structure of the stable compounds gives insight into the fundamental properties of stable compounds. This information is essential to complement the experimental characterization of alkali antimonide samples grown via evaporation techniques that often exhibit metastable or polycrystalline structures.
[1] https://github.com/aim2dat/aim2dat
[2] R. Schier, D. Guo, H.-D. Saßnick, and C. Cocchi, Stability and electronic properties of K-Sb and Na-Sb binary crystals from high-throughput ab initio calculations, submitted (2024).

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