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Stability and electronic properties of CsK2Sb surface facets

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Multi-alkali antimonides have been proposed as a promising class of photocathode materials for particle accelerators. First-principles results have recently complemented the experimental efforts in the characterization of these systems [1]. However, most of the existing studies focus on bulk crystals and still little is known about their surface properties. We fill this gap with an ab initio study based on density-functional theory of the energetic and electronic properties of 7 CsK2Sb surface facets of low Miller index [2]. We analyze the structural optimization of the atomic layers at the interface with vacuum and investigate formation energies as a function of chemical potential to quantify the stability of these systems at varying concentration of the alkali species. We find that the (111)-surfaces terminated with K on top of Sb are generally the most stable ones. The considered surfaces exhibit either semiconducting or metallic character. With a band gap of 1.3 eV for the most stable semiconducting surface and work functions around 2.5 eV for the metallic ones, the computed results are in good agreement with experimental values.

[1] C. Cocchi and H-D. Sassnick, Micromachines 12, 1002 (2021).
[2] R. Schier, H-D. Sassnick, and C. Cocchi, submitted (2022); arXiv:2208.05843.

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