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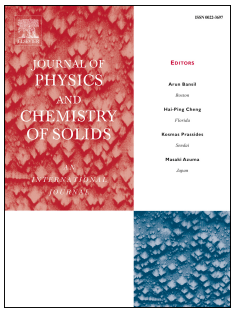

First-principles calculations of different (001) surface terminations of three cubic perovskites $CsCaBr_3$, $CsGeBr_3$, and $CsSnBr_3$

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First-principles calculations of different (001) surface terminations of three cubic perovskites $CsCaBr_3$, $CsGeBr_3$, and $CsSnBr_3$

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Abstract

Three cubic bromide perovskites $CsMBr_3$ (M = Ca, Ge, Sn) with two different surface terminations (CsBr and MBr_2) were studied in this work using the first principles method. A wide range of physical properties, including electronic band structures, atom-projected density of states for each layer, surface relaxation effects, and surface energy, were evaluated for each considered surface termination. Differences between the properties of the bulk and slab models were highlighted. It was shown that surfaces with the CsBr termination have a lower energy and a more pronounced surface rumpling than those with the MBr_2 termination. As a main result of this study, it was demonstrated that the CsBr-terminated surfaces appear to be energetically more stable in each of these three considered perovskites.

Key words: cubic perovskites; first-principles calculations; surface termination.

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