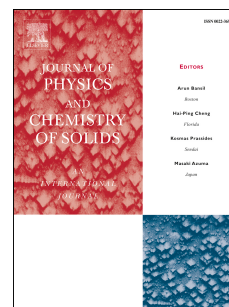


Accepted Manuscript

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PII: S0022-3697(17)31896-6

DOI: [10.1016/j.jpcs.2017.12.052](https://doi.org/10.1016/j.jpcs.2017.12.052)

Reference: PCS 8359

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 7 October 2017

Revised Date: 25 December 2017

Accepted Date: 26 December 2017

Please cite this article as: C.-G. Ma, V. Krasnenko, M.G. Brik, First-principles calculations of different (001) surface terminations of three cubic perovskites CsCaBr₃, CsGeBr₃, and CsSnBr₃, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2017.12.052.

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First-principles calculations of different (001) surface terminations of three cubic perovskites CsCaBr₃, CsGeBr₃, and CsSnBr₃

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Abstract

Three cubic bromide perovskites CsMBr₃ (M = Ca, Ge, Sn) with two different surface terminations (CsBr and MBr₂) 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 MBr₂ 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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