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A lead-free environment-friendly material for optoelectronic and photocatalytic applications: A computational approach

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Abstract

The structural, optoelectronic, and photocatalytic properties of $KCaF_{3-x}Br_x$, where x indicates Br concentration (x=0, 0.6, 1.2, 1.8, 2.4, 3.0), are described here using density functional theory. Computed structural and optoelectronic results for pristine c-$KCaF_3$ are well consistent with existing literature. Bandgap was engineered by impurity inclusion such that the proposed material changes its bandgap for both generalized gradient approximation (GGA) and Heyd, Scuseria, and Ernzerhof hybrid functional (HSE03) formalism from 5.638 eV to 3.807 eV and from 8.538 eV to 2.772 eV respectively. One of the most important criteria for proposing a new end material is structural and mechanical stability, thus the tolerance factor and Born's requirements were used to establish the end materials' stable cubic nature. Optical parameters such as dielectric function, reflection and absorption coefficient, refractive index, and energy loss function are calculated and analyzed up to the photon energy range of 0–35 eV. A redshift was observed whereas the refractive index values for different concentration shows continuous change except for x=2.6. The highest value of reflectivity is observed for $KCaBr_3$ making it useful for several thermoelectric applications. Photocatalytic properties were predicted using a band edge diagram, indicating that the

presented series of materials is a useful candidate for hydrogen evolution reaction (HER), and oxygen evolution reaction (OER). Br substitution at the anionic site of c-$KCaF_3$ has been reported first ever, with promising optical, elastic, and photocatalytic properties that will inspire further research on this material.

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Keywords

Fluoride perovskites; Photocatalysis; Optical properties; Elastic properties; Mechanical properties

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