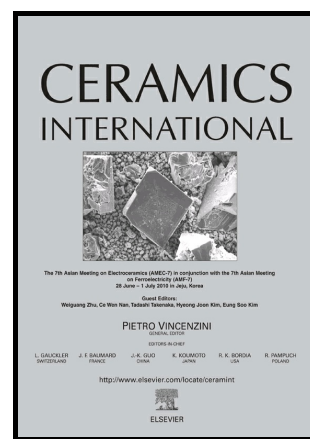


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Structural properties, electronic structures and optical properties of WB₂ with different structures: A theoretical investigation

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Abstract

The structural, electronic and optical properties of six WB₂ diborides with *hP3*, *hP6*, *hP12*, *oP6*, *hR9* and *hR18* structures were systematically investigated using the first-principles calculation based on density functional theory. The optimized atomic coordinates and lattice parameters agree well with the corresponding experimental and theoretical results. All WB₂ are energetically stable, and *hP6*-WB₂ has the best phase stability and *hP3*-WB₂ shows the worst phase stability. The results of density of states and the charge density differences indicate that WB₂ have the strong W-B and B-B covalent bonds. The hardness was obtained from the Mulliken population. The predicted values of absorption coefficient $\alpha(\omega)$ and reflectivity $R(\omega)$ reveal that the laser with a longer wavelength is recommended during the synthesis of WB₂ coatings

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