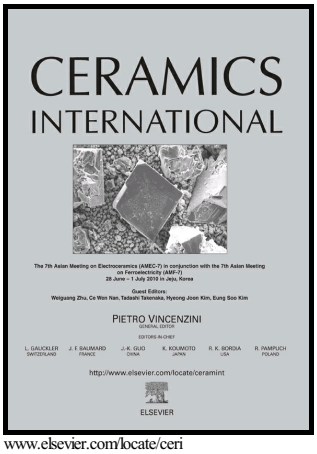

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Structural properties, electronic structures and optical properties of WB_2 with different structures: A theoretical investigation

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Abstract

The structural, electronic and optical properties of six WB_2 diborides with *hP*3, *hP*6, *hP*12, *oP*6, *hR*9 and *hR*18 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 WB_2 are energetically stable, and *hP*6-WB_2 has the best phase stability and *hP*3-WB_2 shows the worst phase stability. The results of density of states and the charge density differences indicate that WB_2 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 WB_2 coatings