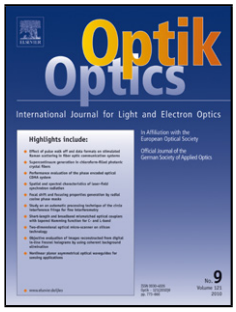

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Electronic and optical properties of beryllium carbide monolayer: First Principles Calculations

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Abstract

New quasi-planar hexacoordinate structure for Be_2C monolayer is studied by the first principles calculations in the framework of the density functional theory. The obtained cohesive energy present a good structural stability for this compound. A direct band gap exist in Γ direction about 1.65 eV, so a semiconducting character is obtained. Optical interband transitions are investigated and described by joint density of states. The optical studies exhibit a transparent character for this compound by 2.5 % reflectivity in the visible range of light. The obtained results suggest this material for nano-electronic devices and applications.

Keywords: Be_2C nanosheet, Gap direction, Optical transitions, Density functional theory.

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