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TWO-DIMENSIONAL STRUCTURES OF THE BERRYLIUM OXIDE: DFT STUDY

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Abstract

First-principles density functional theory calculations were performed in order to investigate the stability and electronic properties of new two-dimensional (2D) Haeckelite BeO structure (containing 8-4 membered rings). The optimized geometry, band-structure, local density of states (LDOS), binding energy, and charge density were calculated. We revealed that BeO Haeckelite structure demonstrates dielectric behaviour and characterizes by an indirect band gap. Furthermore, the influence of the strain on the formation, stability and electronic properties of 2D BeO sheet is discussed.

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