03,05

Half-metallic ferromagnetism and band gap reduction in Cu-doped zinc-blende BeO: first-principle study *

© *L. Kahal*

Département de Génie Physique, Faculté de Physique, Université des Sciences et de la Technologie d'Oran Mohamed Boudiaf, USTO-MB, BP 1505, El M'naouer, 31000 Oran Algérie

E-mail: kahal.larbi@gmail.com, larbi.kahal@univ-usto.dz

(Received August 31, 2016)

In this paper, we report ferromagnetism in copper doped zinc-blende BeO. Our first-principles calculations based on spin density functional theory predicts a total magnetic moment of $1\,\mu_B$ per copper when copper substitutes beryllium in BeO, where $0.58\,\mu_B$ is localized at Cu atom. The results obtained show that the ferromagnetic state is 34 meV lower than the antiferromagnetic state. Calculations indicate an appreciable band gap reduction in BeO. The analysis of the partial density of states reveals that ferromagnetism and reduction of BeO band gap are principally due to the strong $p-d$ coupling of O and Cu.

DOI: 10.21883/FTT.2017.05.44367.337

* Полный текст статьи опубликован в журнале „Physics of the Solid State".