

Abstract Submitted
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Band-gap variations in polytypes of SiC: misleading parameter “hexagonality” and proposal of new parameter YU-ICHIRO MATSUSHITA, ATSUSHI OSHIYAMA, Dept. of Appl. Phy., The University of Tokyo — Silicon carbide (SiC) has been discovered in various polytypes. Each polytype is characterized by its stacking of atomic planes. The band gap varies substantially in each polytype from 2.40 eV to 3.33 eV in spite that the local atomic structures are identical to each other. Recently, we have clarified the mechanism of this intriguing property based on the density functional theory [1]. We have found that the Kohn-Sham orbital at the conduction-band bottom extends broadly in the internal space called channels, and thus floating in the matter. Therefore, important parameter describing the band-gap variations is the channel length, not “hexagonality,” which is thought to be important for the band-gap variations.

[1] Y.-I. Matsushita, S. Furuya, A. Oshiyama, PRL, 108, 246404 (2012).

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