Microscopic mechanism of band-gap variations in SiC polytypes based on *ab initio* calculations: Roles of peculiar electron state floating in internal space

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Silicon Carbide (SiC) is a promising material for power electronic devices. In spite of the vigorous studies for SiC, some unaccountable SiC properties are still remained: Some properties cannot be understood by the conventional semiconductor theories. For example, SiC exhibits hundreds of polytypes, and their structural differences come from the differences of the stacking structures. Though their local atomic structures are identical to each other, their band gaps vary substantially as much as 40%: e.g., 3.33 eV for *2H* (AB-stacking) structure, and 2.40 eV for *3C* (ABC-stacking) structure. The microscopic mechanism of the band-gap variations is lacking, and is remained to be a longstanding problem. We have studied the mechanism, based on the density-functional theory (DFT) calculations.

We have found that the band-gap variation is deeply related to the peculiar electron state at the conduction-band minimum (CBM) [1]. The wave function at the CBM has Nearly-Free-Electron (NFE) like character: The electron state at the CBM distributes not near atomic sites, but extends in internal space broadly, thus *floating* in internal space. Therefore, the energy level of the floating state depends on the electrostatic potential at the interstitial sites, thus showing dramatic variations in band gap in *3C* structure. In addition, we have found that the largeness of the spreading space and its symmetry also have great effects on the changes in band-gap. In fact, we have found that band-gap variations can be completely analyzed by an electron-energy level in the 1-dimensional quantum well with its width being “channel length”, representing the largeness of the spreading space of the floating state. Thus, we have clarified that “channel length” is an essential parameter to describe the band-gap variations [2].

[1] Y. –i. Matsushita, S. Furuya, and A. Oshiyama, PRL, **108**, 246404 (2012).

[2] Y. –i, Matsushita, A. Oshiyama, *in preparation.*