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**Clarification of the relations between stacking structures of $sp^3$ network materials and their band gaps** YU-ICHIRO MATSUSHITA, SHINNOSUKE FURUYA, ATSUSHI OSHIYAMA, The University of Tokyo — Silicon carbide (SiC) has been discovered in various polymorphs. Each polymorph is characterized by its stacking of atomic planes. The band gap varies substantially in each polymorph from 2.40 eV to 3.33 eV in spite that the local atomic structures are identical to each other [1]. The mechanism of this intriguing property have been poorly understood. To clarify the fundamental reasons for this band-gap variation, we have performed the electronic-structure calculations in the density functional theory. We have found that the Kohn-Sham orbital at the conduction-band bottom distributes broadly around the interstitial channel, thus floating in the matter. The way of the floating depends on the stacking of the atomic planes and determines the band gap in each polymorph. We also find that the floating state appears in other $sp^3$-bonded materials, and the band-gap variation is common to the covalent materials. References [1] Properties of Silicon Carbide edited by G. L. Harris (INSPEC, London, 1995).

Yu-ichiro Matsushita
The University of Tokyo

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